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SEARCH REQUEST FORM

Requester's Full Name: S. Kumar Examiner #: 69594 Date: 8/10/06
 Art Unit: 1621 Phone Number: 2-0640 Serial Number: 10 526 327
 Location (Bldg/Room#): REM (Mailbox #): 5C18 Results Format Preferred (circle): PAPER DISK
 *****5C03*****

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following: ME

Title of Invention: Method for the organometallic production of organic intermediates

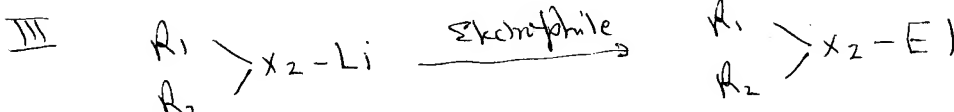
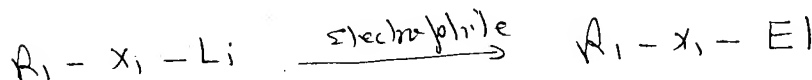
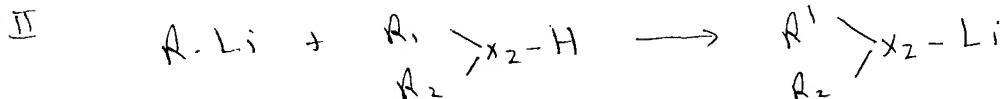
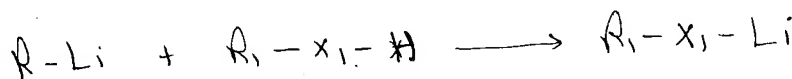
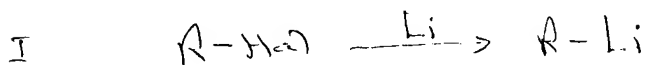
Inventors (please provide full names): Andreas Meudt et al.

Earliest Priority Date: 8/31/02

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.



STAFF USE ONLY

Type of Search

Vendors and cost where applicable

Searcher: _____

____ NA Sequence (#)

____ STN _____ Dialog

Searcher Phone #: _____

____ AA Sequence (#)

____ Questel/Orbit _____ Lexis/Nexis

Searcher Location: _____

____ Structure (#)

____ Westlaw _____ WWW/Internet

Date Searcher Picked Up: _____

____ Bibliographic

____ In-house sequence systems

Date Completed: _____

____ Litigation

____ Commercial _____ Oligomer _____ Score/Length
 ____ Interference _____ SPDI _____ Encode/Transl

Searcher Prep & Review Time: _____

____ Fulltext

____ Other (specify)

Online Time: _____

____ Other

=> d que stat l25

L23 STR

Li^G1 O @3 S @4 N @5
1 2

VAR G1=3/4/5

NODE ATTRIBUTES:

NSPEC IS RC AT 3

NSPEC IS RC AT 4

NSPEC IS RC AT 5

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L25 5136 SEA FILE=REGISTRY SSS/FUL L23

100.0% PROCESSED 87376 ITERATIONS

5136 ANSWERS

SEARCH TIME: 00.00.01

=> d que stat l62

L60 STR

Li^G1 O @3 S @4 N @5
1 2

VAR G1=3/4/5

NODE ATTRIBUTES:

NSPEC IS RC AT 1

NSPEC IS RC AT 3

NSPEC IS RC AT 4

NSPEC IS RC AT 5

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L62 8814 SEA FILE=REGISTRY SSS/FUL L60

100.0% PROCESSED 87376 ITERATIONS

8814 ANSWERS

SEARCH TIME: 00.00.01

=> d que nos l58

L10 QUE ABB=ON PLU=ON AY<2004 OR PY<2004 OR PRY<2004 OR MY
<2004 OR REVIEW/DT
L12 QUE ABB=ON PLU=ON DEPROTON? OR (DE(W) PROTON?)
L13 QUE ABB=ON PLU=ON ELECTROPHIL? OR (ELECTRO(W) PHIL?)
L14 QUE ABB=ON PLU=ON COUPLING
L15 QUE ABB=ON PLU=ON "COUPLING REACTION"+PFT,OLD,NT/CT

L16 QUE ABB=ON PLU=ON LITHIAT? OR LITHIUMIZ? OR LITHIZE?
 L18 QUE ABB=ON PLU=ON LITHIATION+PFT,OLD,NT/CT
 L19 QUE ABB=ON PLU=ON (CARBON(4A)(N OR O OR S OR P OR NITR
 OGEN OR OXYGEN OR SULFUR OR SULPHUR OR PHOSPHORUS OR HETE
 ROATOM OR (HETERO(W)ATOM)))(7A) (BOND? OR ATTACH? OR LINK
 ?)
 L20 QUE ABB=ON PLU=ON FORM OR FORMED OR FORMING OR FORMS O
 R FORMATION OR GENERAT?
 L23 STR
 L25 5136 SEA FILE=REGISTRY SSS FUL L23
 L38 QUE ABB=ON PLU=ON ORGANOLITH? OR (ORGANO(W)LITH?) OR (
 ORGANIC(W)LITH?)
 L41 QUE ABB=ON PLU=ON ARYLLITH? OR ALKYLLITH? OR METHYLLIT
 H? OR ETHYLLITH? OR PROPYLLITH? OR BUTYLLITH? OR ((ARYL O
 R ALKYL OR METHYL OR ETHYL OR PROPYL OR BUTYL) (W) (LI OR L
 ITH?))
 L43 4767 SEA FILE=HCAPLUS ABB=ON PLU=ON L25 (L) RACT/RL
 L44 138 SEA FILE=HCAPLUS ABB=ON PLU=ON L25 (L) (L38 OR L41 OR L16 OR
 L19)
 L45 58 SEA FILE=HCAPLUS ABB=ON PLU=ON L43 AND L44
 L46 61 SEA FILE=HCAPLUS ABB=ON PLU=ON L43 AND (L15 OR L18)
 L47 187 SEA FILE=HCAPLUS ABB=ON PLU=ON (L44 OR L45 OR L46) AND (L12
 OR L13 OR L14 OR L16 OR L19 OR L20 OR L38 OR L41)
 L48 152 SEA FILE=HCAPLUS ABB=ON PLU=ON L47 AND L10
 L49 37 SEA FILE=HCAPLUS ABB=ON PLU=ON (L15 OR L18) (L) L19
 L50 251 SEA FILE=HCAPLUS ABB=ON PLU=ON (L15 OR L18) (L) (L38 OR L41)
 L51 69 SEA FILE=HCAPLUS ABB=ON PLU=ON (L49 OR L50) AND (L12 OR L13)
 L52 62 SEA FILE=HCAPLUS ABB=ON PLU=ON L51 AND L10
 L53 158 SEA FILE=HCAPLUS ABB=ON PLU=ON (L48 OR L52) AND ORGAN?/SC,SX
 L54 25 SEA FILE=HCAPLUS ABB=ON PLU=ON L53 AND L12
 L55 51 SEA FILE=HCAPLUS ABB=ON PLU=ON L53 AND L13
 L58 69 SEA FILE=HCAPLUS ABB=ON PLU=ON L54 OR L55

=> d que nos 178

L10 QUE ABB=ON PLU=ON AY<2004 OR PY<2004 OR PRY<2004 OR MY
 <2004 OR REVIEW/DT
 L12 QUE ABB=ON PLU=ON DEPROTON? OR (DE(W)PROTON?)
 L13 QUE ABB=ON PLU=ON ELECTROPHIL? OR (ELECTRO(W)PHIL?)
 L14 QUE ABB=ON PLU=ON COUPLING
 L15 QUE ABB=ON PLU=ON "COUPLING REACTION"+PFT,OLD,NT/CT
 L16 QUE ABB=ON PLU=ON LITHIAT? OR LITHIUMIZ? OR LITHIZE?
 L18 QUE ABB=ON PLU=ON LITHIATION+PFT,OLD,NT/CT
 L19 QUE ABB=ON PLU=ON (CARBON(4A)(N OR O OR S OR P OR NITR
 OGEN OR OXYGEN OR SULFUR OR SULPHUR OR PHOSPHORUS OR HETE
 ROATOM OR (HETERO(W)ATOM)))(7A) (BOND? OR ATTACH? OR LINK
 ?)
 L20 QUE ABB=ON PLU=ON FORM OR FORMED OR FORMING OR FORMS O
 R FORMATION OR GENERAT?
 L23 STR
 L25 5136 SEA FILE=REGISTRY SSS FUL L23
 L38 QUE ABB=ON PLU=ON ORGANOLITH? OR (ORGANO(W)LITH?) OR (
 ORGANIC(W)LITH?)
 L41 QUE ABB=ON PLU=ON ARYLLITH? OR ALKYLLITH? OR METHYLLIT
 H? OR ETHYLLITH? OR PROPYLLITH? OR BUTYLLITH? OR ((ARYL O
 R ALKYL OR METHYL OR ETHYL OR PROPYL OR BUTYL) (W) (LI OR L
 ITH?))

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L43      4767 SEA FILE=HCAPLUS ABB=ON PLU=ON L25 (L) RACT/RL
L44      138 SEA FILE=HCAPLUS ABB=ON PLU=ON L25 (L) (L38 OR L41 OR L16 OR
          L19)
L45      58 SEA FILE=HCAPLUS ABB=ON PLU=ON L43 AND L44
L46      61 SEA FILE=HCAPLUS ABB=ON PLU=ON L43 AND (L15 OR L18).
L47      187 SEA FILE=HCAPLUS ABB=ON PLU=ON (L44 OR L45 OR L46) AND (L12
          OR L13 OR L14 OR L16 OR L19 OR L20 OR L38 OR L41)
L48      152 SEA FILE=HCAPLUS ABB=ON PLU=ON L47 AND L10
L49      37 SEA FILE=HCAPLUS ABB=ON PLU=ON (L15 OR L18) (L) L19
L50      251 SEA FILE=HCAPLUS ABB=ON PLU=ON (L15 OR L18) (L) (L38 OR L41)

L51      69 SEA FILE=HCAPLUS ABB=ON PLU=ON (L49 OR L50) AND (L12 OR L13)

L52      62 SEA FILE=HCAPLUS ABB=ON PLU=ON L51 AND L10
L53      158 SEA FILE=HCAPLUS ABB=ON PLU=ON (L48 OR L52) AND ORGAN?/SC, SX

L54      25 SEA FILE=HCAPLUS ABB=ON PLU=ON L53 AND L12
L55      51 SEA FILE=HCAPLUS ABB=ON PLU=ON L53 AND L13
L58      69 SEA FILE=HCAPLUS ABB=ON PLU=ON L54 OR L55
L60      STR
L62      8814 SEA FILE=REGISTRY SSS FUL L60
L68      5309 SEA FILE=HCAPLUS ABB=ON PLU=ON L62 (L) (RACT+NT)/RL
L69      376 SEA FILE=HCAPLUS ABB=ON PLU=ON L62 (L) (L14 OR L16 OR L19 OR
          L38 OR L41)
L70      125 SEA FILE=HCAPLUS ABB=ON PLU=ON L68 AND L69
L71      104 SEA FILE=HCAPLUS ABB=ON PLU=ON L69 AND (L15 OR L18)
L72      144 SEA FILE=HCAPLUS ABB=ON PLU=ON (L70 OR L71) AND L10
L73      14 SEA FILE=HCAPLUS ABB=ON PLU=ON L72 AND (L12 OR L13)
L74      3 SEA FILE=HCAPLUS ABB=ON PLU=ON L73 AND (L14 OR L19)
L75      11 SEA FILE=HCAPLUS ABB=ON PLU=ON L73 AND ORGANIC/SC, SX
L76      14 SEA FILE=HCAPLUS ABB=ON PLU=ON (L73 OR L74 OR L75)
L77      2 SEA FILE=HCAPLUS ABB=ON PLU=ON L76 AND L12 AND L13
L78      71 SEA FILE=HCAPLUS ABB=ON PLU=ON L58 OR L77

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=> d que stat 180
L79      STR

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PRO

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RRT      O @3      S @4      N @5      C X G2
Li^G1    6      7
1      2

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VAR G1=3/4/5

VAR G2=3/4/5

NODE ATTRIBUTES:

```

NSPEC    IS RC      AT      1
NSPEC    IS RC      AT      3
NSPEC    IS RC      AT      4
NSPEC    IS RC      AT      5
NSPEC    IS RC      AT      6

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DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE

L80 27 SEA FILE=CASREACT SSS SAM L79 (916 REACTIONS)

4.9% DONE 5000 VERIFIED 916 HIT RXNS 27 DOCS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED VERIFICATIONS: 2007360 TO 2041960
PROJECTED ANSWERS: 13030 TO 16232

=> d que nos 192

L10 QUE ABB=ON PLU=ON AY<2004 OR PY<2004 OR PRY<2004 OR MY
<2004 OR REVIEW/DT
L60 STR
L62 8814 SEA FILE=REGISTRY SSS FUL L60
L82 7715 SEA FILE=CASREACT ABB=ON PLU=ON L62
L84 1756 SEA FILE=CASREACT ABB=ON PLU=ON L82 AND ((COUPLING/BI,AB) OR
(LITHIAT?/BI,AB OR LITHIUMIZ?/BI,AB OR LITHIZE?/BI,AB) OR
((CARBON/BI,AB(4A) (N/BI,AB OR O/BI,AB OR S/BI,AB OR P/BI,AB OR
NITROGEN/BI,AB OR OXYGEN/BI,AB OR SULFUR/BI,AB OR SULPHUR/BI,AB
OR PHOSPHORUS/BI,AB OR HETEROATOM/BI,AB OR (HETERO/BI,AB(W)ATO
M/BI,AB))) (7A) (BOND?/BI,AB OR ATTACH?/BI,AB OR LINK?/BI,AB))
OR (ORGANOLITH?/BI,AB OR (ORGANO/BI,AB(W)LITH?/BI,AB) OR
(ORGANIC/BI,AB(W)LITH?/BI,AB)) OR (ARYLLITH?/BI,AB OR ALKYLLITH?
/BI,AB OR METHYLLITH?/BI,AB OR ETHYLLITH?/BI,AB OR PROPYLLITH?
/BI,AB OR BUTYLLITH?/BI,AB OR ((ARYL/BI,AB OR ALKYL/BI,AB OR
METHYL/BI,AB OR ETHYL/BI,AB OR PROPYL/BI,AB OR BUTYL/BI,AB) (W) (LI/BI,AB OR LITH?/BI,AB)))
L85 94 SEA FILE=CASREACT ABB=ON PLU=ON L84 AND (DEPROTON?/BI,AB OR
(DE/BI,AB(W)PROTON?/BI,AB))
L86 51 SEA FILE=CASREACT ABB=ON PLU=ON L84 AND (ELECTROPHIL?/BI,AB
OR (ELECTRO/BI,AB(W)PHIL?/BI,AB))
L87 5 SEA FILE=CASREACT ABB=ON PLU=ON L85 AND L86
L88 110 SEA FILE=CASREACT ABB=ON PLU=ON (L85 OR L86) AND L10
L89 98 SEA FILE=CASREACT ABB=ON PLU=ON L88 AND ORGANIC/SC,SX
L90 4 SEA FILE=CASREACT ABB=ON PLU=ON L87 AND L88
L91 4 SEA FILE=CASREACT ABB=ON PLU=ON L87 AND L89
L92 4 SEA FILE=CASREACT ABB=ON PLU=ON (L90 OR L91) AND L10

=> d que stat 193

L79 STR

PRO
RRT O @3 S @4 N @5 C X G2
Li ^ G1 6 7
1 2

VAR G1=3/4/5

VAR G2=3/4/5

NODE ATTRIBUTES:

NSPEC	IS RC	AT	1
NSPEC	IS RC	AT	3
NSPEC	IS RC	AT	4
NSPEC	IS RC	AT	5
NSPEC	IS RC	AT	6

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE

L93 43 SEA FILE=CHEMINFORMRX SSS SAM L79 (304 REACTIONS)

12.5% DONE 1000 VERIFIED 304 HIT RXNS 43 DOCS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.10

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED VERIFICATIONS: 155300 TO 165420
PROJECTED ANSWERS: 7558 TO 9992

=> d his l116

(FILE 'USPATFULL, USPAT2' ENTERED AT 10:43:52 ON 23 AUG 2006)

L116 8 S L115 AND L11

=> d que nos l116

L11 QUE ABB=ON PLU=ON AY<2004 OR PY<2004 OR PRY<2004
L12 QUE ABB=ON PLU=ON DEPROTON? OR (DE(W) PROTON?)
L13 QUE ABB=ON PLU=ON ELECTROPHIL? OR (ELECTRO(W) PHIL?)
L14 QUE ABB=ON PLU=ON COUPLING
L16 QUE ABB=ON PLU=ON LITHIAT? OR LITHIUMIZ? OR LITHIZE?
L18 QUE ABB=ON PLU=ON LITHIATION+PFT,OLD,NT/CT
L19 QUE ABB=ON PLU=ON (CARBON(4A) (N OR O OR S OR P OR NITR
OGEN OR OXYGEN OR SULFUR OR SULPHUR OR PHOSPHORUS OR HETE
ROATOM OR (HETERO(W)ATOM)) (7A) (BOND? OR ATTACH? OR LINK
?)
L60 STR
L62 8814 SEA FILE=REGISTRY SSS FUL L60
L63 181 SEA FILE=REGISTRY ABB=ON PLU=ON L62 AND USPATFULL/LC
L64 39 SEA FILE=REGISTRY ABB=ON PLU=ON L62 AND USPAT2/LC
L94 QUE ABB=ON PLU=ON C07F001-02/IPC
L95 QUE ABB=ON PLU=ON C07B?/IPC
L96 QUE ABB=ON PLU=ON (C07B041 OR C07B043 OR C07B045)/IPC
L98 5394 SEA L63 OR L64
L99 5 SEA L98 AND L18
L100 55 SEA L98 AND L16/TI, IT, CC, CT, ST, STP
L101 59 SEA L98 AND L14/TI, IT, CC, CT, ST, STP
L102 135 SEA L14/TI, IT, CC, CT, ST, STP AND L16/TI, IT, CC, CT, ST, STP
L103 234 SEA (L99 OR L100 OR L101 OR L102) AND L11
L104 137 SEA L103 AND L19/TI, IT, CC, CT, ST, STP, BI, AB
L105 26 SEA L103 AND L12/TI, IT, CC, CT, ST, STP, BI, AB
L106 14 SEA L103 AND L13/TI, IT, CC, CT, ST, STP, BI, AB
L107 8 SEA L104 AND L105 AND L106
L108 7 SEA L103 AND L94
L109 10 SEA L103 AND (L95 OR L96)
L112 1 SEA L103 AND L96
L113 1 SEA L108 AND L112
L114 1 SEA L108 AND L109
L115 8 SEA L107 OR (L112 OR L113 OR L114)

L116 8 SEA L115 AND L11

=> d que stat l121
L60 STR

Li^G1 O@3 S@4 N@5
1 2

VAR G1=3/4/5
NODE ATTRIBUTES:
NSPEC IS RC AT 1
NSPEC IS RC AT 3
NSPEC IS RC AT 4
NSPEC IS RC AT 5
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE
L121 0 SEA FILE=WPIX SSS FUL L60

100.0% PROCESSED 1525 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.05

=> d que l124

L94 QUE ABB=ON PLU=ON C07F001-02/IPC
L97 QUE ABB=ON PLU=ON ((N261 OR N262 OR N263) (P) (N341 OR N
342 OR N343 OR N331 OR N332 OR N333 OR N334 OR N335 OR N3
52)) /M0,M1,M2,M3,M4,M5,M6
L122 22 SEA FILE=WPIX ABB=ON PLU=ON L97 AND L94
L123 19 SEA FILE=WPIX ABB=ON PLU=ON L122 AND ((DEPROTON?/BIX OR
(DE/BIX(W) PROTON?/BIX)) OR (ELECTROPHIL?/BIX OR (ELECTRO/BIX(W)
PHIL?/BIX)) OR (COUPLING/BIX) OR (LITHIUM/BIX OR LI/BIX) OR
(LITHIAT?/BIX OR LITHIUMIZ?/BIX OR LITHIZE?/BIX) OR ((CARBON/BI
X(4A) (N/BIX OR O/BIX OR S/BIX OR P/BIX OR NITROGEN/BIX OR
OXYGEN/BIX OR SULFUR/BIX OR SULPHUR/BIX OR PHOSPHORUS/BIX OR
HETEROATOM/BIX OR (HETERO/BIX(W) ATOM/BIX))) (7A) (BOND?/BIX OR
ATTACH?/BIX OR LINK?/BIX)) OR (ORGANOLITH?/BIX OR (ORGANO/BIX(W)
) LITH?/BIX) OR (ORGANIC/BIX(W) LITH?/BIX)) OR (ARYLLITH?/BIX OR
ALKYLLITH?/BIX OR METHYLLITH?/BIX OR ETHYLLITH?/BIX OR
PROPYLLITH?/BIX OR BUTYLLITH?/BIX OR ((ARYL/BIX OR ALKYL/BIX
OR METHYL/BIX OR ETHYL/BIX OR PROPYL/BIX OR BUTYL/BIX) (W) (LI/BI
X OR LITH?/BIX)))
L124 22 SEA FILE=WPIX ABB=ON PLU=ON L122 OR L123

=> d his l137

(FILE 'MEDLINE, BIOSIS, EMBASE' ENTERED AT 11:02:28 ON 23 AUG 2006)
L137 9 S L134-L136

=> d que nos l137

L12 QUE ABB=ON PLU=ON DEPROTON? OR (DE(W) PROTON?)
L13 QUE ABB=ON PLU=ON ELECTROPHIL? OR (ELECTRO(W) PHIL?)

L14 QUE ABB=ON PLU=ON COUPLING
 L16 QUE ABB=ON PLU=ON LITHIAT? OR LITHIUMIZ? OR LITHIZE?
 L19 QUE ABB=ON PLU=ON (CARBON(4A) (N OR O OR S OR P OR NITR
 OGEN OR OXYGEN OR SULFUR OR SULPHUR OR PHOSPHORUS OR HETE
 ROATOM OR (HETERO(W)ATOM)) (7A) (BOND? OR ATTACH? OR LINK
 ?)
 L60 STR
 L62 8814 SEA FILE=REGISTRY SSS FUL L60
 L65 1 SEA FILE=REGISTRY ABB=ON PLU=ON L62 AND MEDLINE/LC
 L66 11 SEA FILE=REGISTRY ABB=ON PLU=ON L62 AND BIOSIS/LC
 L67 1 SEA FILE=REGISTRY ABB=ON PLU=ON L62 AND EMBASE/LC
 L133 126 SEA L65 OR L66 OR L67
 L134 2 SEA L133 AND (L19 OR L14)
 L135 3 SEA L133 AND L16
 L136 6 SEA L133 AND (L12 OR L13)
 L137 9 SEA (L134 OR L135 OR L136)

=> d his l145

(FILE 'MEDLINE, BIOSIS, EMBASE, PASCAL, JICST-EPLUS, JAPIO, CABA,
 LIFESCI, BIOENG, BIOTECHNO, BIOTECHDS, DRUGU, DRUGB, VETU, VETB,
 SCISEARCH, CONFSCI, DISSABS' ENTERED AT 11:06:11 ON 23 AUG 2006)

L145 7 S L144 AND L10
 SAVE TEMP L145 KUM327MUL1B/A

FILE 'STNGUIDE' ENTERED AT 11:22:53 ON 23 AUG 2006

=> d que l145

L10 QUE ABB=ON PLU=ON AY<2004 OR PY<2004 OR PRY<2004 OR MY
 <2004 OR REVIEW/DT
 L12 QUE ABB=ON PLU=ON DEPROTON? OR (DE(W)PROTON?)
 L13 QUE ABB=ON PLU=ON ELECTROPHIL? OR (ELECTRO(W)PHIL?)
 L14 QUE ABB=ON PLU=ON COUPLING
 L16 QUE ABB=ON PLU=ON LITHIAT? OR LITHIUMIZ? OR LITHIZE?
 L17 QUE ABB=ON PLU=ON LITHIUM OR LI
 L19 QUE ABB=ON PLU=ON (CARBON(4A) (N OR O OR S OR P OR NITR
 OGEN OR OXYGEN OR SULFUR OR SULPHUR OR PHOSPHORUS OR HETE
 ROATOM OR (HETERO(W)ATOM)) (7A) (BOND? OR ATTACH? OR LINK
 ?)
 L38 QUE ABB=ON PLU=ON ORGANOLITH? OR (ORGANO(W)LITH?) OR (ORGANIC(W)LITH?)
 L41 QUE ABB=ON PLU=ON ARYLLITH? OR ALKYLITH? OR METHYLLITH?
 H? OR ETHYLLITH? OR PROPYLLITH? OR BUTYLLITH? OR ((ARYL O
 R ALKYL OR METHYL OR ETHYL OR PROPYL OR BUTYL) (W) (LI OR L
 ITH?))
 L142 3180 SEA (L17 OR L16 OR L38 OR L41) (20A) (L19 OR L14)
 L143 49 SEA L142 AND L12
 L144 13 SEA L143 AND L13
 L145 7 SEA L144 AND L10

=> dup rem l78 l58 l92 l116 l124 l137 l145

FILE 'HCAPLUS' ENTERED AT 11:25:37 ON 23 AUG 2006

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PROCESSING COMPLETED FOR L78

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PROCESSING COMPLETED FOR L116

PROCESSING COMPLETED FOR L124

PROCESSING COMPLETED FOR L137

PROCESSING COMPLETED FOR L145

L146 115 DUP REM L78 L58 L92 L116 L124 L137 L145 (75 DUPLICATES REMOVED)

ANSWERS '1-71' FROM FILE HCAPLUS

ANSWERS '72-74' FROM FILE CASREACT

ANSWERS '75-81' FROM FILE USPATFULL

ANSWERS '82-101' FROM FILE WPIX

ANSWER '102' FROM FILE MEDLINE

ANSWERS '103-111' FROM FILE BIOSIS

ANSWER '112' FROM FILE SCISEARCH

ANSWERS '113-115' FROM FILE DISSABS

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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Aug 18, 2006 (20060818/UP).

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YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CASREACT, USPATFULL, WPIX, MEDLINE, BIOSIS, SCISEARCH, DISSABS' - CONTINUE? (Y)/N:y

L146 ANSWER 1 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 1
 ACCESSION NUMBER: 2004:198231 HCAPLUS
 DOCUMENT NUMBER: 140:253710
 TITLE: preparation of aryllithium compounds using lithium metal and their reaction with electrophiles.
 INVENTOR(S): Meudt, Andreas; Lehnemann, Bernd; Erbes, Michael; Forstinger, Klaus
 PATENT ASSIGNEE(S): Clariant G.m.b.H., Germany
 SOURCE: Ger. Offen., 10 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10240262	A1	20040311	DE 2002-10240262	20020831 <--
WO 2004024738	A1	20040325	WO 2003-EP9252	20030821 <--
W: BR, CA, CN, IN, JP, KR, NO, RU, SG, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
EP 1537126	A1	20050608	EP 2003-794907	20030821 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2006131762	A1	20060622	US 2005-526237	20050228 <--
PRIORITY APPLN. INFO.:			DE 2002-10240262	A 20020831 <--
			WO 2003-EP9252	W 20030821 <--

OTHER SOURCE(S): CASREACT 140:253710; MARPAT 140:253710

ED Entered STN: 11 Mar 2004

AB Aryllithium compds. [I, II; Q = Li; R1-R4 = H, Me, (substituted) alkyl, alkoxy, alkylamino, (substituted) Ph, etc.; X1-X4 = C, N; adjoining pairs of X1-X4 = O, S, NH, etc.; Z = CF3, OCF3, Cl, F, alkoxy, aryloxy, alkylthio, arylthio, CH2OH, etc.], were prepared by reaction of Ar-Hal [Ar = (substituted) Ph, naphthyl, biphenyl; Hal = F, Cl, Br, iodo] with Li to give Ar-Li and reaction of Ar-Li with I, II; (Q = H; other variables as above). The resulting aryllithium compds. were reacted with electrophiles to give I, II (Q = electrophile residue; other variables as above). Thus, 4-ClC6H4Me and furfural di-Et acetal were added to a mixture of Li metal and cat. biphenyl in THF at -65° over 1.5 h; after 9 h tri-Me borate was added over 30 min. followed by stirring for another 30 min. and addition of aqueous HCl to give 81.5% 5-formylfuran-2-boronic acid.

IC ICM C07F001-02

ICS C07F005-02; C07B037-04; C07B041-00

CC 29-4 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 25, 27

ST aryllithium reaction electrophile; formylfuranboronate methoxyphenylboronate chlorotrifluoromethylbenzoate trifluoromethylchlorobenzaldehyde difluoroacetophenone furylboronate prepn; lithiation aryl halide lithium metal

IT Nitriles, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

- and (aliphatic nitriles; preparation of aryllithium compds. using lithium metal and their reaction with **electrophiles**)
- IT Nitriles, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(aromatic; preparation of aryllithium compds. using lithium metal and their reaction with **electrophiles**)
- IT **Electrophiles**
(boron **electrophiles**; preparation of aryllithium compds. using lithium metal and their reaction with **electrophiles**)
- IT Aromatic hydrocarbons, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(halo; preparation of aryllithium compds. using lithium metal and their reaction with **electrophiles**)
- IT Nitro compounds
RL: RCT (Reactant); RACT (Reactant or reagent)
(nitroenolates; preparation of aryllithium compds. using lithium metal and their reaction with **electrophiles**)
- IT Alkylating agents, biological
Coupling reaction
Lithiation
(preparation of aryllithium compds. using lithium metal and their reaction with **electrophiles**)
- IT Aldehydes, reactions
Amides, reactions
Cyanates
Epoxides
Esters, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aryllithium compds. using lithium metal and their reaction with **electrophiles**)
- IT Sulfonic acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(salts, acyl; preparation of aryllithium compds. using lithium metal and their reaction with **electrophiles**)
- IT Carboxylic acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(salts; preparation of aryllithium compds. using lithium metal and their reaction with **electrophiles**)
- IT Aldehydes, reactions
Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(α,β -unsatd.; preparation of aryllithium compds. using lithium metal and their reaction with **electrophiles**)
- IT 37181-39-8D, Triflate, derivs
RL: RCT (Reactant); RACT (Reactant or reagent)
(aryl triflates; preparation of aryllithium compds. using lithium metal and their reaction with **electrophiles**)
- IT 92-52-4, Biphenyl, uses
RL: CAT (Catalyst use); USES (Uses)
(preparation of aryllithium compds. using lithium metal and their reaction with **electrophiles**)
- IT 2376-00-3P 13331-23-2P, 2-Furylboronic acid 13670-99-0P,
2,6-Difluoroacetophenone 23112-96-1P, 2,6-Dimethoxyphenylboronic acid
27329-70-0P, 5-Formylfuran-2-boronic acid 60611-22-5P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of aryllithium compds. using lithium metal and their reaction with **electrophiles**)
- IT 75-21-8, Oxirane, reactions 98-15-7, 3-Chlorobenzotrifluoride

107-31-3, Methyl formate 108-24-7, Acetic anhydride 110-00-9, Furan
 121-43-7, Trimethyl borate 124-38-9, Carbon dioxide, reactions
 151-10-0, Resorcinol dimethyl ether 372-18-9, 1,3-Difluorobenzene
 463-51-4, Ketene 630-08-0, Carbon monoxide, reactions 2053-29-4,
 Azomethine 13529-27-6, Furfural diethyl acetal 28963-72-6D, Immonium,
 salts

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of aryllithium compds. using lithium metal and their reaction
 with electrophiles)

IT 106-43-4, p-Chlorotoluene 108-90-7, Chlorobenzene, reactions

7439-93-2, Lithium, reactions 25168-05-2, Chlorotoluene

RL: RGT (Reagent); RACT (Reactant or reagent)

(preparation of aryllithium compds. using lithium metal and their reaction
 with electrophiles)

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YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CASREACT, USPATFULL, WPIX, MEDLINE,
 BIOSIS, SCISEARCH, DISSABS' - CONTINUE? (Y)/N:y

L146 ANSWER 2 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2004:198230 HCAPLUS

DOCUMENT NUMBER: 140:253342

TITLE: Preparation of derivatized aromatics using
 organolithium reagents prepared in situ.

INVENTOR(S): Meudt, Andreas; Lehnemann, Bernd; Erbes, Michael;
 Forstinger, Klaus

PATENT ASSIGNEE(S): Clariant G.m.b.H., Germany

SOURCE: Ger. Offen., 9 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10240261	A1	20040311	DE 2002-10240261	20020831 <--
WO 2004024663	A1	20040325	WO 2003-EP9251	20030821 <--

W: BR, CA, CN, IN, JP, KR, NO, RU, SG, US

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,

IT, LU, MC, NL, PT, RO, SE, SI, SK, TR

PRIORITY APPLN. INFO.: DE 2002-10240261 A 20020831 <--

OTHER SOURCE(S): CASREACT 140:253342; MARPAT 140:253342

ED Entered STN: 11 Mar 2004

AB Title compds. [I; R1-R5 = H, M, (cyclic) (substituted) alkyl, alkoxy,
 alkylamino, arylamino, Ph, heteroaryl, alkylthio, arylthio,
 diarylphosphino, etc.; 2 neighboring R1-R5 = atoms to form a condensed
 ring; X1-X5 = C, N; Q = electrophile residue], were prepared by
 treatment of Ar-Hal [Ar = (substituted) Ph, pyridyl, naphthyl; Hal = F,
 Cl, Br, iodo] with Li to give Ar-Li in situ, reaction of the latter with I
 (Q = Hal; other variables as above) to give I (Q = Li; other variables as
 above), and treatment of the latter with an electrophile. Thus,
 Li in THF at -35° was treated with 4-ClC6H4Me and cat. biphenyl
 followed by stirring for 5 h; the mixture was cooled to -70° and
 treated with 4-BrC6H4CF3. After stirring for 2 h at -50°, Ac2O in
 THF was added at -30° followed by stirring for 30 min. to give
 87.2% 4-trifluoromethylacetophenone.

IC ICM C07F001-02
ICS C07B037-04; C04B041-00
CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **Lithiation**
(lithiation of aryl halides; preparation of derivatized aroms. using **organolithium** reagents prepared in situ)
IT **Coupling reaction**
Electrophiles
(preparation of derivatized aroms. using **organolithium** reagents prepared in situ)

L146 ANSWER 3 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2004:198229 HCAPLUS
DOCUMENT NUMBER: 140:253119
TITLE: Preparation of organic compounds containing carbon-heteroatom bonds using organolithium reagents prepared in situ.
INVENTOR(S): Meudt, Andreas; Lehnemann, Bernd; Erbes, Michael; Forstinger, Klaus
PATENT ASSIGNEE(S): Clariant G.m.b.H., Germany
SOURCE: Ger. Offen., 9 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10240260	A1	20040311	DE 2002-10240260	20020831 <--
WO 2004024737	A1	20040325	WO 2003-EP9250	20030821 <--
W: BR, CA, CN, IN, JP, KR, NO, RU, SG, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
EP 1537125	A1	20050608	EP 2003-794905	20030821 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005537331	T2	20051208	JP 2004-535121	20030821 <--
US 2005258553	A1	20051124	US 2005-526327	20050228 <--
PRIORITY APPLN. INFO.:			DE 2002-10240260	A 20020831 <--
			WO 2003-EP9250	W 20030821 <--

OTHER SOURCE(S): CASREACT 140:253119; MARPAT 140:253119

ED Entered STN: 11 Mar 2004

AB A process for formation of carbon-heteroatom bonds comprises (1) treatment of R-Hal (R = Me, (substituted) alkyl, cycloalkyl, Ph, aryl, heteroaryl; Hal = F, Cl, Br, iodo) with Li metal to give RLi, (2) use of RLi for **deprotonation** of R1X1H or R1R2X2H [X1 = O, S, sp²-hybridized N; X2 = sp³-hybridized N; R1, R2 = H, Me, (substituted) alkyl, alkenyl, alkynyl, acyl, alkoxy, aryloxy, dialkylamino, arylamino, heteroaryl, carboxylate, etc.; R1R2 = atoms to form a ring], and (3) treatment of R1X1Li or R1R2X2Li with a carbon **electrophile**. Thus, Li in THF at -35° was treated with 4-ClC6H4Me followed by stirring for ca. 8 h; 2-furylmethanol was added followed by warming to room temperature, addition of propargyl bromide, and reflux for 2 h to give 93% 2-furylmethyl propargyl ether.

IC ICM C07B037-04
ICS C07B041-00; C07B043-00; C07B045-00
CC 21-2 (General Organic Chemistry)
Section cross-reference(s): 23, 25, 27

IT Coupling reaction

Lithiation

(preparation of organic compds. containing carbon-heteroatom bonds using organolithium reagents prepared in situ)

L146 ANSWER 4 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 4

ACCESSION NUMBER: 2005:155125 HCAPLUS

DOCUMENT NUMBER: 143:477420

TITLE: Asymmetric deprotonation with
alkyllithium-(-)-sparteine

AUTHOR(S): Hoppe, Dieter; Christoph, Guido

CORPORATE SOURCE: Organisch-Chemisches Institut, Westfaelischen
Wilhelms-Universitaet Muenster, Muenster, D-48149,
GermanySOURCE: Chemistry of Organolithium Compounds (2004), Volume 2,
1055-1164. Editor(s): Rappoport, Zvi; Marek, Ilan.
John Wiley & Sons Ltd.: Chichester, UK.
CODEN: 69GMVM; ISBN: 0-470-84339-X

DOCUMENT TYPE: Conference; General Review

LANGUAGE: English

ED Entered STN: 24 Feb 2005

AB A review on asym. deprotonation. Several different procedures
for asym. deprotonation using alkyllithiums and sparteine is
covered in this overview.

CC 21-0 (General Organic Chemistry)

ST review asym deprotonation alkyllithium sparteine

IT Amines, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)
(allyl; asym. deprotonation with alkyllithium-(-)-sparteine)

IT Asymmetric synthesis and induction

Desymmetrization

(asym. deprotonation with alkyllithium-(-)-sparteine)

IT Epoxides

RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. deprotonation with alkyllithium-(-)-sparteine)

IT Deprotonation

Lithiation

(asym.; asym. deprotonation with alkyllithium
-(-)-sparteine)

IT Ethers, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)
(benzyl; asym. deprotonation with alkyllithium-(-)-sparteine)

IT Resolution (separation)

(kinetic; asym. deprotonation with alkyllithium-(-)-
sparteine)

IT Heterocyclic compounds

RL: RCT (Reactant); RACT (Reactant or reagent)
(nitrogen; asym. deprotonation with alkyllithium-(-)-
sparteine)

IT Addition reaction

Aldol condensation

(stereoselective; asym. deprotonation with
alkyllithium-(-)-sparteine)

IT 90-39-1, (-)-Sparteine

RL: RGT (Reagent); RACT (Reactant or reagent)
(asym. deprotonation with alkyllithium-(-)-sparteine)REFERENCE COUNT: 413 THERE ARE 413 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L146 ANSWER 5 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 6

ACCESSION NUMBER: 2003:900371 HCAPLUS

DOCUMENT NUMBER: 140:128452

TITLE: Stereoselective lithiation of α,β -epoxy- γ,δ -vinylsilanes and transformation into α -silylated ketones

AUTHOR(S): Courillon, Christine; Marie, Jean-Charle; Malacria, Max

CORPORATE SOURCE: Laboratoire de Chimie Organique, Universite P. et M. Curie, Associe au CNRS, Paris, 75252, Fr.

SOURCE: Tetrahedron (2003), 59(49), 9759-9766

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:128452

ED Entered STN: 18 Nov 2003

AB A (cis) α,β -epoxy- γ,δ -vinyl-silane undergoes lithiation α to the Si atom with retention of the configuration of the oxirane. This leads to new silylated vinyloxiranes with a quaternary silylated stereogenic C atom. The possible and efficient rearrangement of a Me substituted adduct into a β,γ -unsatd.- α -silylated ketone is shown.

CC 29-6 (Organometallic and Organometalloidal Compounds)

ST epoxyvinylsilane prepn stereoselective **electrophilic** trapping reaction; ketones alpha silylated prepn; vinyloxiranes silylated prepn

IT **Lithiation**
(ring opening reactions of alpha,beta-epoxyvinylsilanes with **alkyllithiums**)

IT Asymmetric synthesis and induction

Silylation

Stereoselective synthesis

(stereoselective **electrophilic** trapping reactions of alpha,beta-epoxyvinylsilanes and their transformation into alpha-silylated ketones)

IT Ketones, preparation

RL: SPN (Synthetic preparation); PREP (Preparation)

(stereoselective **electrophilic** trapping reactions of alpha,beta-epoxyvinylsilanes and their transformation into alpha-silylated ketones)

IT Epoxides

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(vinyloxiranes; stereoselective **electrophilic** trapping reactions of alpha,beta-epoxyvinylsilanes and their transformation into alpha-silylated ketones)

IT Silanes

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(vinylsilanes, α,β -epoxy- γ,δ -vinylsilanes; stereoselective **electrophilic** trapping reactions of alpha,beta-epoxyvinylsilanes and their transformation into alpha-silylated ketones)

IT 1779-49-3, Methyltriphenylphosphonium bromide

RL: RCT (Reactant); RACT (Reactant or reagent)

(Wittig reaction of phosphonium bromide with silylated aldehyde to give alpha,beta-epoxyvinylsilanes and their subsequent stereoselective **electrophilic** trapping reactions)

IT 1067-74-9 88738-78-7

- RL: RCT (Reactant); RACT (Reactant or reagent)
(Wittig reaction of silylated aldehyde with phosphonium bromide to give alpha,beta-epoxyvinylsilanes and their subsequent stereoselective electrophilic trapping reactions)
- IT 120789-51-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydride reduction of silylated propargylic alc. to give alpha,beta-epoxyvinylsilanes and their subsequent stereoselective electrophilic trapping reactions)
- IT 630403-40-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Wittig reaction of silylated aldehyde with phosphonium bromide to give alpha,beta-epoxyvinylsilanes and their subsequent stereoselective electrophilic trapping reactions)
- IT 154673-67-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and epoxidn. of silylallylic alc. to give alpha,beta-epoxyvinylsilane and its subsequent stereoselective electrophilic trapping reactions)
- IT 650638-84-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of silylallylic alc. to give alpha,beta-epoxyvinylsilane and its subsequent stereoselective electrophilic trapping reactions)
- IT 75-77-4, Trimethylsilyl chloride, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and stereoselective electrophilic trapping reactions of alpha,beta-epoxyvinylsilanes and their transformation into alpha-silylated ketones)
- IT 444120-55-2P 444120-62-1P 444120-63-2P 650638-87-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and stereoselective electrophilic trapping reactions of alpha,beta-epoxyvinylsilanes and their transformation into alpha-silylated ketones)
- IT 444120-54-1P 444120-57-4P 444120-58-5P 650638-86-1P 650638-88-3P 650638-89-4P 650638-90-7P 650638-95-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and stereoselective electrophilic trapping reactions of alpha,beta-epoxyvinylsilanes and their transformation into alpha-silylated ketones)
- IT 100-52-7, Benzaldehyde, reactions 556-56-9, Allyl iodide 17640-15-2, Methyl cyanoformate
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective electrophilic trapping reactions of alpha,beta-epoxyvinylsilanes and their transformation into alpha-silylated ketones)
- IT 444120-71-2P 444120-72-3P 444120-73-4P 444120-74-5P 650638-85-0P 650638-94-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective electrophilic trapping reactions of alpha,beta-epoxyvinylsilanes and their transformation into alpha-silylated ketones)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2003:545291 HCAPLUS
DOCUMENT NUMBER: 139:245621
TITLE: Ketone Enolization with Lithium Dialkylamides: The Effects of Structure, Solvation, and Mixed Aggregates with Excess **Butyllithium**
AUTHOR(S): Pratt, Lawrence M.; Newman, Anthony; St. Cyr, Jason; Johnson, Harry; Miles, Benjamin; Lattier, April; Austin, Elizabeth; Henderson, Susan; Hershey, Brad; Lin, Ming; Balamraju, Yuvaraju; Sammonds, Laurel; Cheramie, Jeffery; Karnes, Jonathan; Hymel, Ellen; Woodford, Brittini; Carter, Carl
CORPORATE SOURCE: Department of Chemistry, Fisk University, Nashville, TN, 37208, USA
SOURCE: Journal of Organic Chemistry (2003), 68(16), 6387-6391
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

ED Entered STN: 17 Jul 2003

AB The effects of Li dialkylamide structure, mixed aggregate **formation**, and solvation on the stereoselectivity of ketone enolization were examined. Of the Li dialkylamides examined, Li tetramethylpiperidine (LiTMP) in THF resulted in the best enolization selectivity. The stereoselectivity was further improved in the presence of a LiTMP-**butyllithium** mixed aggregate. The use of less polar solvents reduced the enolization stereoselectivity. Ab initio calcns. predict LDA and LiTMP to **form** mixed cyclic dimers in ethereal solvents. The calcns. also predict LiTMP-**alkyllithium** mixed aggregates to competitively inhibit the **formation** of less stereoselective LiTMP-Li enolate mixed aggregates.

CC 22-12 (Physical Organic Chemistry)

Section cross-reference(s): 29

ST ketone enolization lithium dialkylamide MO structure solvation aggregate **butyllithium**; mixed dimer lithium dialkylamide **butyllithium** ketone enolization

IT Density functional theory

(B3LYP; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)

IT Self-consistent reaction field

(CPCM; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)

IT Ethers, reactions

RL: NUU (Other use, unclassified); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)

(coordinating solvents; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)

IT Dimers

RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent) (cyclic mixed; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)

IT Enolization

Hartree-Fock method

Molecular association

- Solvation
Solvent effect
(effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT Ketones, reactions
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT Diastereomers
(geometric, enol; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT Stereochemistry
(geometric; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT Deprotonation
(ketones by lithium reagents; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT Addition reaction
(limited **butyllithium** or aggregate addns. to acetophenone; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT Dimerization enthalpy
(mixed dimers; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT Steric effects
(on mixed aggregate **formation**; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT Molecular structure
(optimized; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT Amines, reactions
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(salts, lithium dialkylamides; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT Free energy
(solvation; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT Free energy
(total; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT NMR (nuclear magnetic resonance)
(⁶Li; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT 108-18-9, Diisopropylamine 768-66-1, 2,2,6,6-Tetramethylpiperidine 999-97-3, 1,1,1,3,3,3-Hexamethyldisilazane
RL: RCT (Reactant); RACT (Reactant or reagent)
(N-lithiation; effects of structure, solvation, and mixed

- aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT 110-18-9, TMEDA
RL: NUU (Other use, unclassified); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(coordinating ligand; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT 60-29-7, Diethyl ether, reactions 109-99-9, THF, reactions
RL: NUU (Other use, unclassified); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(coordinating solvent ligand; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT 75-77-4, Chlorotrimethylsilane, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(derivatization of lithium enolates; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT 521085-98-3 596828-54-5 596828-55-6
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(dimerization with **ethylithium** di-Me etherate; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT 596828-56-7
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(dimerization with lithium dialkylamide di-Me etherate; effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT 4039-32-1 4111-54-0 7439-93-2D, Lithium, tetramethylpiperidine-Et lithium, diisopropylamine-Bu lithium and hexamethyldisilazane-Bu lithium mixed aggregate complexes 14258-72-1D, Lithium-6, tetramethylpiperidine-15N-Et lithium mixed aggregate complexes, reactions 137003-47-5D, lithium-6-Et lithium mixed aggregate complexes 596828-60-3 596828-61-4 596828-62-5 596828-63-6
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT 109-72-8, **Butyllithium**, reactions 811-49-4, **Ethylithium** 38227-87-1
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT 98-86-2, Acetophenone, reactions
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT 51425-53-7 51425-54-8
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(effects of structure, solvation, and mixed aggregates with excess **butyllithium** on ketone enolization with lithium dialkylamides)
- IT 74016-27-6
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM

(Formation, nonpreparative); RACT (Reactant or reagent)
 (effects of structure, solvation, and mixed aggregates with excess
butyllithium on ketone enolization with lithium dialkylamides)

IT 107-87-9, 2-Pentanone

RL: CPS (Chemical process); PEP (Physical, engineering or chemical
 process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant
 or reagent)

(geometric stereochem. of **deprotonation**; effects of
 structure, solvation, and mixed aggregates with excess
butyllithium on ketone enolization with lithium dialkylamides)

IT 596828-57-8 596828-58-9 596828-59-0 596828-64-7
 596828-65-8 596828-66-9

RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical,
 engineering or chemical process); PRP (Properties); RCT (Reactant); FORM
 (Formation, nonpreparative); PROC (Process); **RACT (Reactant or
 reagent)**

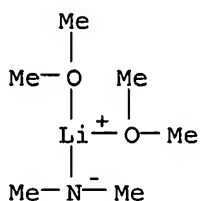
(interconversion of cyclic and open dimers; effects of structure,
 solvation, and mixed aggregates with excess **butyllithium** on
 ketone enolization with lithium dialkylamides)

IT 521085-98-3 596828-54-5 596828-55-6

RL: PRP (Properties); RCT (Reactant); **RACT (Reactant or reagent)**
 (dimerization with **ethylithium** di-Me etherate; effects of
 structure, solvation, and mixed aggregates with excess
butyllithium on ketone enolization with lithium dialkylamides)

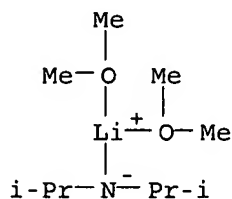
RN 521085-98-3 HCAPLUS

CN Lithium, (N-methylmethanaminato)bis[oxybis[methane]] - (9CI) (CA INDEX
 NAME)



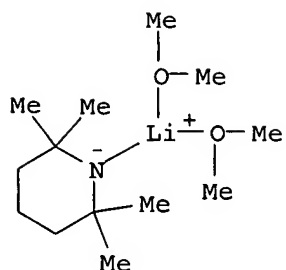
RN 596828-54-5 HCAPLUS

CN Lithium, [N-(1-methylethyl)-2-propanaminato]bis[oxybis[methane]] - (9CI)
 (CA INDEX NAME)



RN 596828-55-6 HCAPLUS

CN Lithium, bis[oxybis[methane]](2,2,6,6-tetramethyl-1-piperidinyl) - (9CI)
 (CA INDEX NAME)



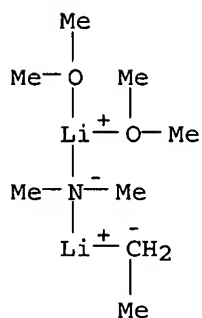
IT 596828-64-7 596828-65-8 596828-66-9

RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)

(interconversion of cyclic and open dimers; effects of structure, solvation, and mixed aggregates with excess butyllithium on ketone enolization with lithium dialkylamides)

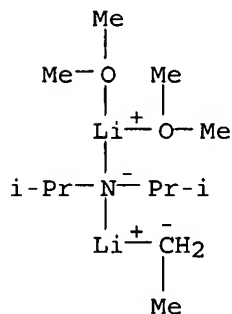
RN 596828-64-7 HCAPLUS

CN Lithium, ethyl[μ-(N-methylmethanaminato)]bis[oxybis[methane]]di- (9CI)
(CA INDEX NAME)



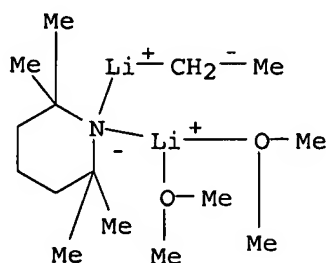
RN 596828-65-8 HCAPLUS

CN Lithium, ethyl[μ-[N-(1-methylethyl)-2-propanaminato]]bis[oxybis[methane]]di- (9CI) (CA INDEX NAME)



RN 596828-66-9 HCAPLUS

CN Lithium, ethylbis[oxybis[methane]][μ-(2,2,6,6-tetramethyl-1-piperidiny)]di- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 7 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 8
 ACCESSION NUMBER: 2003:552700 HCAPLUS
 DOCUMENT NUMBER: 139:364400
 TITLE: Direct transformation of allylic and benzylic thiols, thioethers, and disulfides into organolithium compounds
 AUTHOR(S): Yus, Miguel; Martinez, Pedro; Guijarro, David
 CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de Ciencias, Universidad de Alicante, Alicante, Spain
 SOURCE: Synthetic Communications (2003), 33(13), 2365-2376
 CODEN: SYNCAV; ISSN: 0039-7911
 PUBLISHER: Marcel Dekker, Inc.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:364400
 ED Entered STN: 20 Jul 2003
 AB The reaction of allylic and benzylic thiols, disulfides, and thioethers with excess lithium and a catalytic amount of 4,4'-di-tert-butylbiphenyl (5 mol %) afforded allylic and benzylic organolithium reagents via reductive cleavage of the carbon-sulfur bond. The generated organolithium compds. gave the expected products by reaction with several **electrophiles**, followed by hydrolysis with water. The reaction conditions and the lithiation procedure (stepwise or Barbier-type process) depended on the starting sulfur containing compound
 CC 21-2 (General Organic Chemistry)
 ST lithium reaction allylic benzylic thiol thioether disulfide; organolithium compd reaction **electrophile**
 IT **Lithiation**
 (transformation of allylic and benzylic thiols, thioethers, and disulfides into **organolithium** compds. and subsequent reaction with **electrophiles**)
 IT 75-77-4, Chlorotrimethylsilane, reactions 96-22-0, 3-Pentanone 100-52-7, Benzaldehyde, reactions 100-53-8, Benzyl thiol 108-94-1, Cyclohexanone, reactions 123-19-3, Dipropyl ketone 150-60-7, Dibenzyl disulfide 538-74-9, Dibenzyl sulfide 630-19-3, Pivalaldehyde 766-92-7, Benzyl methyl sulfide 10152-76-8, Allyl methyl sulfide 39067-82-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (transformation of allylic and benzylic thiols, thioethers, and disulfides into organolithium compds. and subsequent reaction with **electrophiles**)
 IT 614-29-9P 770-09-2P, Benzyltrimethylsilane 936-58-3P 1944-01-0P 34577-40-7P 50695-92-6P 62108-07-0P 78055-70-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(transformation of allylic and benzylic thiols, thioethers, and
disulfides into organolithium compds. and subsequent reaction with
electrophiles)

REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 8 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 9

ACCESSION NUMBER: 2003:491897 HCAPLUS

DOCUMENT NUMBER: 140:27720

TITLE: Intramolecular carbolithiation reactions for the
preparation of 3-alkenylpyrrolidines

AUTHOR(S): Coldham, Iain; Price, Kathy N.; Rathmell, Richard E.

CORPORATE SOURCE: School of Chemistry, University of Exeter, Exeter, EX4
4QD, UK

SOURCE: Organic & Biomolecular Chemistry (2003),
1(12), 2111-2119

CODEN: OBCRAK; ISSN: 1477-0520

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:27720

ED Entered STN: 29 Jun 2003

AB Tin-lithium exchange allows the formation of α -amino-organolithium
species, e.g., I, that undergo anionic cyclization onto allylic ethers to
give 3-alkenylpyrrolidines, e.g., II. The methodol. has been applied to
the synthesis of an advanced intermediate related to the natural product
(-)- α -kainic acid III.

CC 27-10 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 26

IT **Lithiation**

Stereoselective synthesis

(preparation of alkenylpyrrolidines via tin-lithium exchange of
 α -amino-organotin species with **butyllithium** followed by
intramol. anionic cyclization onto allylic ethers)

IT 541-41-3, Ethyl chloroformate

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of N-carboxylate derivative of azabicyclic octane via
electrophilic substitution of the corresponding N-benzyl
bicyclic amine with Et chloroformate)

IT 634180-90-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of N-carboxylate derivative of azabicyclic octane via
electrophilic substitution of the corresponding N-benzyl
bicyclic amine with Et chloroformate)

REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 9 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 10

ACCESSION NUMBER: 2003:347338 HCAPLUS

DOCUMENT NUMBER: 139:100899

TITLE: Selectivities in Reactions of Organolithium Reagents
with Unprotected 2-Halobenzoic Acids

AUTHOR(S): Gohier, Frederic; Castanet, Anne-Sophie; Mortier,
Jacques

CORPORATE SOURCE: Unite de Chimie Organique Moleculaire et
Macromoleculaire (UMR 6011), Faculte des Sciences,
Universite du Maine and CNRS, Le Mans, 72085, Fr.

SOURCE: Organic Letters (2003), 5(11), 1919-1922

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:100899

ED Entered STN: 08 May 2003

AB Exposing 2-FC6H4CO2H to 2.2 equiv of LTMP at ca. -78 °C leads to **deprotonation** at the 3-position whereas 2-ClC6H4CO2H and 2-BrC6H4CO2H are lithiated adjacent to the carboxylate. The resulting dianions are trapped as such by chlorotrimethylsilane. In the absence of internal quench, the 6-lithio derivs. isomerize to the more stable 3-lithio derivs. The latter eliminate lithium halide and set free benzyne-3-carboxylate that reacts regioselectively with LTMP to give 3-tetramethylpiperidinobenzoic acid.

CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT **Lithiation**

(regioselective; selectivities in reactions of **organolithium** reagents with unprotected 2-halobenzoic acids)

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 10 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 11

ACCESSION NUMBER: 2003:496720 HCAPLUS

DOCUMENT NUMBER: 140:128137

TITLE: Variations in the solid-state, solution and theoretical structures of a laterally **deprotonated** aromatic tertiary amide

AUTHOR(S): Armstrong, David R.; Clayden, Jonathan; Haigh, Robert; Linton, David J.; Schooler, Paul; Wheatley, Andrew E. H.

CORPORATE SOURCE: Department of Pure and Applied Chemistry, University of Strathclyde, Strathclyde, G1 1XL, UK

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2003), (14), 1694-1695

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:128137

ED Entered STN: 30 Jun 2003

AB Reaction of 2-ethyl-N,N-diisopropyl-1-naphthamide 3 with ButLi in THF affords a laterally metalated derivative which exists as a tris(thf) solvated monomer with no Li-C interaction and an sp² hybridized carbanionic center in the solid-state; NMR spectroscopy suggests that this structure is viable in solution but that Li-C bonded atropisomers are also possible and calcns. corroborate these data.

CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 22, 75

ST solid soln theor structure laterally **deprotonated** arom tertiary amide; **lithiated** ethyldiisopropyl naphthamide solid soln theor structure; crystal mol structure **lithiated** ethyldiisopropyl naphthamide

IT Density functional theory

(B3LYP; variations in solid-state, solution and theor. structures of **lithiated** ethyldiisopropyl naphthamide as an laterally **deprotonated** aromatic tertiary amide)

IT Crystal structure

Molecular structure

(of **lithiated** ethyldiisopropyl naphthamide)

IT Molecular structure
(optimized; variations in solid-state, solution and theor. structures of
lithiated ethyldiisopropyl naphthamide as an laterally
deprotonated aromatic tertiary amide)

IT Atropisomers
Solution structure
Total energy
(variations in solid-state, solution and theor. structures of
lithiated ethyldiisopropyl naphthamide as an laterally
deprotonated aromatic tertiary amide)

IT 189389-39-7 651003-88-2 651003-90-6 651003-91-7 651003-92-8
651003-93-9 651003-94-0 651003-95-1 651003-96-2 651003-97-3
651003-98-4 651003-99-5
RL: CPS (Chemical process); PEP (Physical, engineering or chemical
process); PRP (Properties); PROC (Process)
(B3LYP calcn.; variations in solid-state, solution and theor. structures
of **lithiated ethyldiisopropyl naphthamide** as an laterally
deprotonated aromatic tertiary amide)

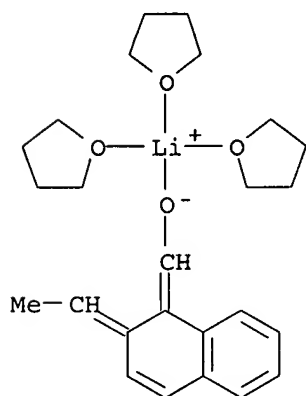
IT 651003-89-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; variations in solid-state, solution and theor.
structures of **lithiated ethyldiisopropyl naphthamide** as an
laterally **deprotonated aromatic tertiary amide**)

IT 189389-35-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(variations in solid-state, solution and theor. structures of
lithiated ethyldiisopropyl naphthamide as an laterally
deprotonated aromatic tertiary amide)

IT 651003-89-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; variations in solid-state, solution and theor.
structures of **lithiated ethyldiisopropyl naphthamide** as an
laterally **deprotonated aromatic tertiary amide**)

RN 651003-89-3 HCAPLUS

CN Lithium, [[(2E)-2-ethylidene-1(2H)-naphthalenyldiene]methanolato]tris(tetr
ahydrofuran)-, (T-4)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 11 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 12
ACCESSION NUMBER: 2004:265907 HCAPLUS
DOCUMENT NUMBER: 141:295663

TITLE: Synthesis of diarylmethylamines via electrophilic trapping of tricarbonyl chromium complexed aryllithium intermediates with imines

AUTHOR(S): Chen, Yong-Jun; Zhao, Cui-Hua; Liu, Li; Wang, Dong

CORPORATE SOURCE: Laboratory of Chemical Biology, Chinese Academy of Sciences, Beijing, 100080, Peop. Rep. China

SOURCE: Journal of Chemical Research, Synopses (2003), (11), 740-743

CODEN: JRPSDC; ISSN: 0308-2342

PUBLISHER: Science Reviews

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:295663

ED Entered STN: 01 Apr 2004

AB Diarylmethylamine derivs., e.g. I, were synthesized in good yields via lithiation of the tricarbonyl(η^6 -arene)chromium complexes, e.g. II, followed by electrophilic trapping with imines, e.g. Ph-CH=NTs, and de-complexation (sunlight and air).

CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 29

ST photochem electrophilic coupling imine lithiation carbonyl chromium aryllithium prep

IT Amines, preparation

RL: SPN (Synthetic preparation); PREP (Preparation)
(aromatic; synthesis of diarylmethylamines via electrophilic trapping of tricarbonyl chromium complexed aryllithium intermediates with imines)

IT Coupling reaction
(photochem.; synthesis of diarylmethylamines via electrophilic trapping of tricarbonyl chromium complexed aryllithium intermediates with imines)

IT Imines

RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of diarylmethylamines via electrophilic trapping of tricarbonyl chromium complexed aryllithium intermediates with imines)

IT 783-08-4 3157-65-1 12082-02-9 12082-03-0 12082-05-2 12082-08-5,
(Benzene)tricarbonylchromium 12083-24-8 12116-44-8 13707-41-0
13707-46-5 14674-38-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of diarylmethylamines via electrophilic trapping of tricarbonyl chromium complexed aryllithium intermediates with imines)

IT 853-83-8P 224784-33-2P 258277-17-7P 258277-19-9P 258277-20-2P
765315-92-2P 765315-96-6P 765315-97-7P 765315-98-8P 765315-99-9P
765316-00-5P 765316-01-6P 765316-02-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of diarylmethylamines via electrophilic trapping of tricarbonyl chromium complexed aryllithium intermediates with imines)

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 12 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 13

ACCESSION NUMBER: 2003:79499 HCAPLUS

DOCUMENT NUMBER: 139:6948

TITLE: Sequestered alkyllithiums: why phenyllithium alone is suitable for betaine-ylide generation

AUTHOR(S): Wang, Qian; Deredas, Dariusz; Huynh, Cyril; Schlosser,

Manfred
CORPORATE SOURCE: Institut de Chimie Organique, Universite, BCh,
Lausanne, 1015, Switz.
SOURCE: Chemistry--A European Journal (2003), 9(2),
570-574
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:6948

ED Entered STN: 02 Feb 2003

AB The key step in the trans-selective modification of the Wittig reaction is the α -lithiation of the lithium bromide coordinated ylide-aldehyde adduct (the so-called "P-betaine"). The olefination reactions were carried out for RCHO and [R1CH2PPh3]Br (R = C6H5, Ph, CH2:CMc, iPr, tBu; R1 = Bu, Pr, PhCH2CH2, C5H11) applying PhLi, MeLi, BuLi, sec-BuLi and tert-BuLi as bases. Only PhLi and MeLi yielded (E)-alkenes with good stereoselectivity (>98%), whereas other organolithium bases yielded (E)-(Z)-mixts. Special experiment with (C6D5)3P showed, that phenyllithium acts solely as base, forming α -lithiated betaine, and no P-Ph addition intermediates were formed. Only phenyllithium effects this **deprotonation** rapidly and cleanly. Alkylolithiums (in particular, butyl-, sec-butyl-, and tert-butyllithium) react only sluggishly and incompletely, being tied up in very stable mixed aggregates with the lithium alkoxide part of the betaines. The different results of the Wittig reaction are accounted to the low aggregation ability of PhLi and (MeLi)4, which disfavors the formation of mixed product-base aggregates.

CC 29-7 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22, 23

ST phenyllithium alkylolithium Wittig reaction trans selective mechanism; phosphonium salt **deprotonation** phenyllithium methyllithium butyllithium mechanism aggregation; trans selectivity olefination aldehyde triphenylphosphonium salt phenyllithium alkylolithium base

IT **Lithiation**

(Wittig olefination intermediate; mechanism of lithiation of aldehyde-ylide adduct in trans-selective Wittig olefination with salt-containing **organolithium** bases)

IT **Deprotonation**

(Wittig olefination intermediate; mechanism of trans-selective Wittig olefination with salt-containing organolithium bases in dependence on their structure)

IT Phosphonium compounds

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent) (**deprotonation** of phosphonium salts in mechanism of trans-selective Wittig olefination with salt-containing organolithium bases)

IT 1779-51-7, Butyltriphenylphosphonium bromide 4762-26-9, Hexyltriphenylphosphonium bromide 7484-37-9, Triphenyl(3-phenylpropyl)phosphonium bromide 21406-61-1, Pentyltriphenylphosphonium bromide

RL: RCT (Reactant); RACT (Reactant or reagent) (**deprotonation**, olefination; stereoselectivity and mechanism of trans-selective Wittig olefination of aldehydes with salt-containing organolithium bases)

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 13 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 14

ACCESSION NUMBER: 2003:321596 HCAPLUS
 DOCUMENT NUMBER: 140:27851
 TITLE: Configurational stability of chiral **lithiated** cyclopropyl nitriles: A density functional study
 AUTHOR(S): Carlier, Paul R.
 CORPORATE SOURCE: Department of Chemistry, Virginia Tech, Blacksburg, VA, 24061, USA
 SOURCE: Chirality (2003), 15(4), 340-347
 CODEN: CHRLEP; ISSN: 0899-0042
 PUBLISHER: Wiley-Liss, Inc.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

ED Entered STN: 27 Apr 2003

AB Chiral, configurationally stable **lithiated** nitriles would be valuable intermediates for asym. C-C bond-forming reactions. To gain insight into the design of such species, Walborsky's attempted enantioselective **deprotonation**/trapping reactions of a chiral cyclopropyl nitrile were studied computationally up to the MP2(fc)/6-31+G* and B3LYP/6-31+G* levels. Study of cyclopropyl nitrile/LiNH₂ **deprotonation** transition structures demonstrated a significant (20-23 kcal/mol) kinetic preference for N-**lithiation**, and a facile (4-6 kcal/mol barrier) conducted tour racemization pathway for the N-**lithiated** nitrile product. Addition of a model directing group (formyl) to the β -C of the cyclopropyl ring is predicted to significantly favor C-**lithiation** over N-**lithiation**, both kinetically and thermodynamically. Thus, chiral β -Lewis base substituted cyclopropyl nitriles may serve as precursors to chiral, configurationally stable **organolithium** reagents.

CC 29-2 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22

ST DFT study configurational stability chiral **lithiated** cyclopropyl nitrile; inversion barrier chiral **lithiated** cyclopropyl nitrile DFT; **deprotonation** mechanism chiral cyclopropyl nitrile lithium amide DFT

IT Density functional theory
 (B3LYP; DFT study of configurational stability of chiral **lithiated** cyclopropyl nitriles and **deprotonation** mechanisms for cyclopropyl nitriles)

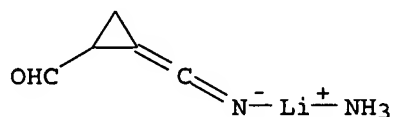
IT Inversion barrier
 Total energy
 Transition state structure
 (DFT study of configurational stability of chiral **lithiated** cyclopropyl nitriles and **deprotonation** mechanisms for cyclopropyl nitriles)

IT MP2 (second-order Moller-Plesset method)
 (MP2(fc); DFT study of configurational stability of chiral **lithiated** cyclopropyl nitriles and **deprotonation** mechanisms for cyclopropyl nitriles)

IT Nitriles, properties
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
 (cyclopropyl nitriles; DFT study of configurational stability of chiral **lithiated** cyclopropyl nitriles and **deprotonation** mechanisms for cyclopropyl nitriles)

IT **Deprotonation**
 Racemization
 (mechanism; DFT study of configurational stability of chiral **lithiated** cyclopropyl nitriles and **deprotonation** mechanisms for cyclopropyl nitriles)

- IT Molecular structure
(optimized; DFT study of configurational stability of chiral lithiated cyclopropyl nitriles and deprotonation mechanisms for cyclopropyl nitriles)
- IT **Deprotonation**
(stereoselective, mechanism; DFT study of configurational stability of chiral lithiated cyclopropyl nitriles and deprotonation mechanisms for cyclopropyl nitriles)
- IT 633303-93-2 633304-01-5 633304-02-6 633304-03-7
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)
(DFT study of configurational stability of chiral lithiated cyclopropyl nitriles and deprotonation mechanisms for cyclopropyl nitriles)
- IT 633303-88-5 633303-91-0 633303-97-6
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); **RACT (Reactant or reagent)**
(DFT study of configurational stability of chiral lithiated cyclopropyl nitriles and deprotonation mechanisms for cyclopropyl nitriles)
- IT 5500-21-0, Cyclopropyl nitrile 7782-89-0, Lithium amide 633303-86-3
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); **RACT (Reactant or reagent)**
(DFT study of configurational stability of chiral lithiated cyclopropyl nitriles and deprotonation mechanisms for cyclopropyl nitriles)
- IT 633303-95-4
RL: PRP (Properties)
(DFT study of configurational stability of chiral lithiated cyclopropyl nitriles and deprotonation mechanisms for cyclopropyl nitriles)
- IT 633303-99-8
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); **RACT (Reactant or reagent)**
(hydrogen-bonded isomers; DFT study of configurational stability of chiral lithiated cyclopropyl nitriles and deprotonation mechanisms for cyclopropyl nitriles)
- IT 1724-45-4, Cyclopropane ion(1-) 21438-99-3, Acetonitrile ion(1-), properties 76510-29-7, Cyclopropanecarbonitrile ion(1-)
RL: PRP (Properties)
(inversion barrier, deformation angle; DFT study of configurational stability of chiral lithiated cyclopropyl nitriles and deprotonation mechanisms for cyclopropyl nitriles)
- IT 633304-01-5
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)
(DFT study of configurational stability of chiral lithiated cyclopropyl nitriles and deprotonation mechanisms for cyclopropyl nitriles)
- RN 633304-01-5 HCAPLUS
- CN Lithium, ammine[(carbonimidoyl-κN)cyclopropanecarboxaldehydato]-(9CI) (CA INDEX NAME)



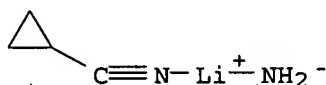
IT 633303-88-5 633303-91-0 633303-97-6

RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); **RACT (Reactant or reagent)**

(DFT study of configurational stability of chiral lithiated cyclopropylnitriles and deprotonation mechanisms for cyclopropylnitriles)

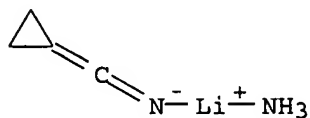
RN 633303-88-5 HCAPLUS

CN Lithium, amido(cyclopropanecarbonitrile)- (9CI) (CA INDEX NAME)



RN 633303-91-0 HCAPLUS

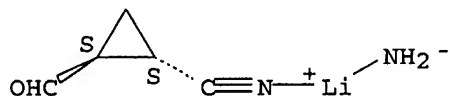
CN Lithium, ammine(1-cyclopropylidenemethaniminato)- (9CI) (CA INDEX NAME)



RN 633303-97-6 HCAPLUS

CN Lithium, amido[rel-(1R,2R)-2-formylcyclopropanecarbonitrile-κN]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 7782-89-0, Lithium amide

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); **RACT (Reactant or reagent)**

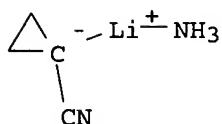
(DFT study of configurational stability of chiral lithiated cyclopropylnitriles and deprotonation mechanisms for cyclopropylnitriles)

RN 7782-89-0 HCAPLUS

CN Lithium amide (Li(NH2)) (7CI, 8CI, 9CI) (CA INDEX NAME)

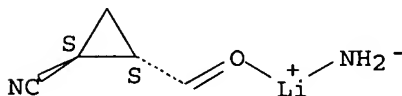
Li-NH2

IT 633303-95-4
 RL: PRP (Properties)
 (DFT study of configurational stability of chiral lithiated
 cyclopropyl nitriles and deprotonation mechanisms for
 cyclopropyl nitriles)
 RN 633303-95-4 HCAPLUS
 CN Lithium, ammine(1-cyanocyclopropyl)- (9CI) (CA INDEX NAME)



IT 633303-99-8
 RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical,
 engineering or chemical process); PRP (Properties); RCT (Reactant); FORM
 (Formation, nonpreparative); PROC (Process); RACT (Reactant or
 reagent)
 (hydrogen-bonded isomers; DFT study of configurational stability of
 chiral lithiated cyclopropyl nitriles and
 deprotonation mechanisms for cyclopropyl nitriles)
 RN 633303-99-8 HCAPLUS
 CN Lithium, amido[rel-(1R,2R)-2-(formyl-κO)cyclopropanecarbonitrile]-
 (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 14 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 15
 ACCESSION NUMBER: 2003:580605 HCAPLUS
 DOCUMENT NUMBER: 140:128102
 TITLE: The palladium-catalyzed cross-coupling reaction of
 lithium polyfluorophenyltrimethoxyborates with
 4-fluoroiodobenzene
 AUTHOR(S): Frohn, Hermann-Josef; Adonin, Nicolay Yu.; Bardin,
 Vadim V.; Starichenko, Vladimir F.
 CORPORATE SOURCE: Inorganic Chemistry, Institute of Chemistry,
 University Duisburg-Essen, Duisburg, D-47048, Germany
 SOURCE: Journal of Fluorine Chemistry (2003),
 122(2), 195-199
 CODEN: JFLCAR; ISSN: 0022-1139
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 140:128102
 ED Entered STN: 30 Jul 2003
 AB Li[C6F5B(OMe)3], Li[C6HF4B(OMe)3] (all three isomers) and
 Li[3,4,5-C6H2F3B(OMe)3] are examples of polyfluorophenyltrimethoxyborate

salts, which have been used as reagents in Pd-catalyzed cross-coupling reactions. A series of polyfluorinated biphenyls C₆H₅-nFn-C₆H₄F-4', e.g., I, were obtained from Li[C₆H₅-nFnB(OMe)₃] and the model substrate 4-FC₆H₄I in the presence of Pd catalysts. The influence of the number and the position of fluorine atoms in the polyfluorophenyltrimethoxyborate salts on the reactivity in the coupling reaction was elucidated.

CC 25-8 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT Aromatic compounds

RL: RCT (Reactant); RACT (Reactant or reagent)

(fluoro arenes; preparation of polyfluorinated biphenyls via **deprotonation** of polyfluorobenzenes with butyllithium followed by addition to tri-Me borate and palladium-catalyzed cross-coupling with fluoriodobenzene)

IT Cross-coupling reaction

(preparation of polyfluorinated biphenyls via **deprotonation** of polyfluorobenzenes with butyllithium followed by addition to tri-Me borate and palladium-catalyzed cross-coupling with fluoriodobenzene)

IT Borates

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of polyfluorinated biphenyls via **deprotonation** of polyfluorobenzenes with butyllithium followed by addition to tri-Me borate and palladium-catalyzed cross-coupling with fluoriodobenzene)

IT Biaryls

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of polyfluorinated biphenyls via **deprotonation** of polyfluorobenzenes with butyllithium followed by addition to tri-Me borate and palladium-catalyzed cross-coupling with fluoriodobenzene)

IT 3375-31-3, Palladium(II)acetate 14221-01-3,

Tetrakis(triphenylphosphine)palladium

RL: CAT (Catalyst use); USES (Uses)

(preparation of polyfluorinated biphenyls via **deprotonation** of polyfluorobenzenes with butyllithium followed by addition to tri-Me borate and palladium-catalyzed cross-coupling with fluoriodobenzene)

IT 121-43-7, Trimethylborate 327-54-8, 2,3,5,6-Tetrafluorobenzene

352-34-1, 4-Fluoriodobenzene 363-72-4, Pentafluorobenzene 551-62-2, 2,3,4,5-Tetrafluorobenzene 2367-82-0, 1,2,3,5-Tetrafluorobenzene

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of polyfluorinated biphenyls via **deprotonation** of polyfluorobenzenes with butyllithium followed by addition to tri-Me borate and palladium-catalyzed cross-coupling with fluoriodobenzene)

IT 408497-69-8P 649756-92-3P 649756-93-4P 649756-94-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of polyfluorinated biphenyls via **deprotonation** of polyfluorobenzenes with butyllithium followed by addition to tri-Me borate and palladium-catalyzed cross-coupling with fluoriodobenzene)

IT 29778-93-6P 505058-31-1P 505058-33-3P 505058-35-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of polyfluorinated biphenyls via **deprotonation** of polyfluorobenzenes with butyllithium followed by addition to tri-Me borate and palladium-catalyzed cross-coupling with fluoriodobenzene)

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 15 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 16
ACCESSION NUMBER: 2003:684684 HCAPLUS
DOCUMENT NUMBER: 140:76663

TITLE: (-)-Sparteine mediated lithiation of
N-BOC-N-p-(methoxyphenyl) allylic amines and conjugate
addition to nitroalkenes: scope, reaction pathway, and
synthetic applications
AUTHOR(S): Johnson, Timothy Allen
CORPORATE SOURCE: Univ. of Illinois, Urbana, IL, USA
SOURCE: (2002) 267 pp. Avail.: UMI, Order No.
DA3070342
From: Diss. Abstr. Int., B 2003, 63(11), 5250
DOCUMENT TYPE: Dissertation
LANGUAGE: English
ED Entered STN: 02 Sep 2003
AB Unavailable
CC 21-2 (General Organic Chemistry)
IT Deprotonation
Lithiation
(stereoselective; scope, reaction pathway, and synthetic applications
of the conjugate addition of **organolithium** reagents generated by
(-)-sparteine-mediated lithiation of N-BOC-N-p-(methoxyphenyl) allylic
amines to nitroalkenes)

L146 ANSWER 16 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 17
ACCESSION NUMBER: 2002:456574 HCAPLUS
DOCUMENT NUMBER: 137:352700
TITLE: Six- and five-membered 3-alkoxy-2-lithiocycloalkenes:
new stable non-anionic β -functionalized
organolithium compounds
AUTHOR(S): Yus, Miguel; Ramon, Diego J.; Gomez, Inmaculada
CORPORATE SOURCE: Facultad de Ciencias, Departamento de Quimica
Organica, Universidad de Alicante, Alicante, E-03080,
Spain
SOURCE: Tetrahedron (2002), 58(25), 5163-5172
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:352700
ED Entered STN: 18 Jun 2002
AB Naphthalene-catalyzed reductive lithiation of various functionalized
chlorocycloalkenes leads to the corresponding non-anionic
 β -alkoxyfunctionalized organolithium reagents. Their reaction with
different **electrophiles**, such as water, aldehydes, ketones and
imines, gave the expected products. The diastereoselection in the
reaction with aldehydes can be modified by the use of different additives.
In the case of using 3-methoxy-2-chlorocyclopentene as starting material,
and depending on reaction time, unexpected bicyclopentadiene derivs. were
isolated, together with the expected compds.
CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 29
IT **Electrophiles**
(effect of reactive **electrophiles** on synthesis of stable
nonanionic β -functionalized organolithium compds. based on six-
and five-membered 3-alkoxy-2-lithiocycloalkenes)
IT **Lithiation**
Lithiation catalysts
(reductive; synthesis of stable nonanionic β -functionalized
organolithium compds. based on six- and five-membered
3-alkoxy-2-lithiocycloalkenes via naphthalene-catalyzed reductive
lithiation)
IT 96-22-0, Diethyl ketone 98-86-2, Methyl phenyl ketone, reactions

100-52-7, Benzaldehyde, reactions 108-94-1, Cyclohexanone, reactions
120-92-3, Cyclopentanone 630-19-3 1013-88-3, Benzophenone imine
7732-18-5, Water, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(**electrophile**; effect of reactive **electrophiles** on
synthesis of stable nonanionic β -functionalized organolithium
compds. based on six- and five-membered 3-alkoxy-2-lithiocycloalkenes)

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 17 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 18

ACCESSION NUMBER: 2002:456541 HCAPLUS

DOCUMENT NUMBER: 137:279224

TITLE: Reductive lithiation of cyclic benzofused ethers: a
source of oxygen-functionalized organolithium
compounds

AUTHOR(S): Yus, Miguel; Foubelo, Francisco; Ferrandez, Jose V.;
Bachki, Abderrazak

CORPORATE SOURCE: Facultad de Ciencias, Departamento de Quimica
Organica, Universidad de Alicante, Alicante, E-03080,
Spain

SOURCE: Tetrahedron (2002), 58(24), 4907-4915

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:279224

ED Entered STN: 18 Jun 2002

AB The reaction of 2,3-dihydrobenzofuran (1) with Li and a catalytic amount of
4,4'-di-tert-butylbiphenyl (DTBB, 5%) in THF at 0° for 1.5 h,
followed by addition of an **electrophile** [$E^+ = H_2O$, $tBuCHO$,
 $PhCH_2CHO$, $Ph(CH_2)_2CHO$, $PhCHO$, furfural, Me_2CO , Et_2CO , cyclopentanone,
cyclohexanone, cyclooctanone, (-)-menthone] in THF at -78° gives,
after hydrolysis, diol compds., 2-HOC $6H_4CH_2CH_2(E)$, 3. Some diols 3, e.g.,
2-HOC $6H_4CH_2CH_2CR_1R_2OH$ [$R_1 = H$, $R_2 = Ph$; $R_1 = R_2 = Et$; $R_1R_2 = (CH_2)_n$, $n =$
5, 7] are easily transformed into 2-substituted chromans I under acidic
reaction conditions. The reductive lithiation of chroman I ($R_1 = R_2 = H$)
at 20° for 3 h leads exclusively to the intermediate 8, which is
formed through a dearylation process, and isomerizes to the apparently
more stable benzylic intermediate 9. The reaction of these intermediates
with different **electrophiles** [$E^+ = tBuCHO$, $PhCHO$, furfural,
 Me_2CO , $[CH_3(CH_2)_4]_2CO$, cyclopentanone, cyclohexanone, (-)-menthone,
 Ph_2CO], at -78° in THF leads, after hydrolysis, to a mixture of
regioisomers 2-(E) $C_6H_4(CH_2)_3OH$ 10 and $PhCH(E)CH_2CH_2OH$ 11. The reaction of
2,3-benzofuran (12) with an excess of Li and a catalytic amount of DTBB (5%)
in THF at 0° for 45 min leads to dianionic intermediate 13 through
a dealkylation process, which after hydrolysis gives 2-vinylphenol 14. In
the case of 4H-chromene (15), reductive opening was performed at
20° for 45 min, a mixture of dearylation and dealkylation
intermediates 16 and 17, resp., was obtained (2:1 ratio) giving, after
hydrolysis, 3-phenylpropanal (18) and 2-allylphenol (19).

CC 29-2 (Organometallic and Organometalloidal
Compounds)

ST benzofused ether cyclic reductive lithiation addn **electrophile**;
chroman substituted prepn reductive lithiation ring opening; diol
benzofused prepn dehydration cyclization reaction phosphoric acid

IT **Electrophiles**

(addition reaction to lithiated cyclic benzofused ethers)

IT **Lithiation**

(of cyclic benzofused ethers to give oxygen-functionalized

organolithium compds.)
IT Addition reaction
(reductive lithiation of cyclic benzofused ethers to give oxygen-functionalized organolithium compds. and subsequent addition with electrophiles)
IT 368859-68-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate formation and reaction with electrophiles)
IT 254-03-5, 4H-1-Benzopyran 271-89-6, Benzofuran 493-08-3 496-16-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(sequential reductive lithiation and addition reactions with electrophiles)

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 18 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 19
ACCESSION NUMBER: 2002:149677 HCAPLUS
DOCUMENT NUMBER: 137:63434
TITLE: 'meso-Selective' functionalisation of N-benzyl- α -methylbenzylamine derivatives by α -lithiation and alkylation
AUTHOR(S): Bragg, Ryan A.; Clayden, Jonathan; Menet, Christel J.
CORPORATE SOURCE: Department of Chemistry, University of Manchester, Manchester, M13 9PL, UK
SOURCE: Tetrahedron Letters (2002), 43(11), 1955-1959
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:63434

ED Entered STN: 27 Feb 2002
AB Lithiation and methylation of amide and carbamate derivs. of α -methylbenzylamine proceeds with high diastereoselectivity in favor of meso bis- α -methylbenzylamine derivs. Carboxylation of the intermediate organolithium is also diastereoselective, and with N-Boc p-methoxy- α -methylbenzylamine as starting material, oxidative cleavage provides a new asym. route to phenylglycine. Other electrophiles give a range of stereochem. outcomes, apparently depending on the stereospecificity of their reactions with a pair of diastereoisomeric organolithiums of low to moderate configurational stability.
CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 21
IT Asymmetric synthesis and induction
Carboxylation
Lithiation
Methylation
Stereochemistry
Transmetalation

(preparation of phenylglycines via diastereoselective reactions of organolithium methylbenzylamine derivs.)
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 19 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 20
ACCESSION NUMBER: 2002:114418 HCAPLUS
DOCUMENT NUMBER: 136:309813
TITLE: Dearomatizing Annulation of Five-Membered Rings to

Naphthalenes by Organolithium Cyclization
AUTHOR(S): Clayden, Jonathan; Kenworthy, Martin N.
CORPORATE SOURCE: Department of Chemistry, University of Manchester,
Manchester, M13 9PL, UK
SOURCE: Organic Letters (2002), 4(5), 787-790
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:309813
ED Entered STN: 13 Feb 2002
AB γ -Lithiopropyl naphthalenes and their oxa- and aza-tethered analogs
cyclize by nucleophilic addition of the organolithium to the naphthalene
ring. The resulting benzyllithiums react stereoselectively with
electrophiles to give dearomatized tricyclic products with
structural similarity to the aryl naphthalene lignans.
CC 27-7 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 26
ST aryl naphthalene lignan analog naphthofuran prepn; benzindanone prepn;
lithiopropyl naphthalene cyclization dearomatization **electrophile**
substitution
IT Cyclization
Lithiation
Substitution reaction, **electrophilic**
(dearomatizing annelation of five-membered rings to naphthalenes by
organolithium cyclization)
REFERENCE COUNT: 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 20 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 21
ACCESSION NUMBER: 2002:266004 HCAPLUS
DOCUMENT NUMBER: 137:154719
TITLE: Efficient mono- and dilithiation of
2-bromo-1,1-diphenylethene with n-
butyllithium/tetramethylethylenediamine
AUTHOR(S): Korneev, Sergei M.; Kaufmann, Dieter E.
CORPORATE SOURCE: Institute of Chemistry, St. Petersburg State
University, St. Petersburg, 198504, Russia
SOURCE: Synthesis (2002), (4), 491-496
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:154719
ED Entered STN: 10 Apr 2002
AB Lithiation of 2-bromo-1,1-diphenylethene with BuLi or Me₃CLi-TMEDA in
pentane at -100 °C effects a halogen-lithium exchange to give
2-lithio-1,1-diphenylethene exclusively, which reacts with
electrophiles to provide 2-substituted-1,1-diphenylethenes in high
yields. Further lithiation of the monolithium derivative with BuLi-TMEDA
results in the direct ortho-lithiation of the 2-located benzene ring to
give dilithium derivative which forms disubstituted ethenes or heterocycles on
treatment with **electrophiles**. Me₃CLi-TMEDA is ineffective for
the second lithiation step.
CC 25-3 (Benzene, Its Derivatives, and Condensed Benzenoid
Compounds)
IT **Lithiation**
(efficient mono- and dilithiation of 2-bromo-1,1-diphenylethene with
butyllithium-tetramethylethylenediamine)
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS

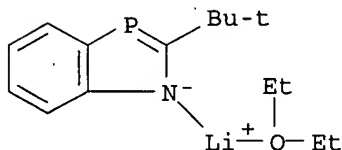
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 21 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 22
ACCESSION NUMBER: 2002:219037 HCAPLUS
DOCUMENT NUMBER: 137:6234
TITLE: Enhanced leaving ability of methoxy group and retarded **deprotonation** on the carbon atom linked to the 1-position of 8-phosphino- or 8-amino-naphthalene
AUTHOR(S): Toshimitsu, Akio; Saeki, Tomoyuki; Tamao, Kohei
CORPORATE SOURCE: Institute for Chemical Research, Kyoto University, Kyoto, 611-0011, Japan
SOURCE: Chemistry Letters (2002), (3), 278-279
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:6234
ED Entered STN: 22 Mar 2002
AB In an attempt to lithiate a benzylic C, a benzyl Me ether bearing an 8-phosphino-1-naphthyl group at the benzylic C (I) is treated with t-butyllithium to gave a quite unexpected compound, e.g., II, arising not from **deprotonation** but from the removal of the methoxy group accompanied by the introduction of two t-Bu groups into the naphthalene ring.
CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 75
ST selective **deprotonation** benzyl carbon lithiation benzylmethylether contg phosphinonaphthyl group; methoxy group enhanced leaving ability lithiation benzylmethylether contg phosphinonaphthyl; crystal structure phosphino methylene tertbutyl tetrahydronaphthalene; mol structure phosphino methylene tertbutyl tetrahydronaphthalene
IT Methoxy group
(enhanced leaving ability of methoxy group and retarded **deprotonation** on the benzyl carbon atom of benzyl Me ether containing of phosphino- or aminonaphthyl group upon reaction with organolithium reagent)
IT Ethers, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(enhanced leaving ability of methoxy group and retarded **deprotonation** on the benzyl carbon atom of benzyl Me ether containing of phosphino- or aminonaphthyl group upon reaction with organolithium reagent)
IT Lithiation
(regioselective; enhanced leaving ability of methoxy group and retarded **deprotonation** on the benzyl carbon atom of benzyl Me ether containing of phosphino- or aminonaphthyl group upon reaction with organolithium reagent)
IT Deprotonation
(retarded; enhanced leaving ability of methoxy group and retarded **deprotonation** on the benzyl carbon atom of benzyl Me ether containing of phosphino- or aminonaphthyl group upon reaction with organolithium reagent)
IT 403804-06-8 433710-09-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(tert-butyllithium-promoted **deprotonation** reaction)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 22 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 23

ACCESSION NUMBER: 2002:175873 HCAPLUS
 DOCUMENT NUMBER: 137:109320
 TITLE: Metalated 1,3-azaphospholes: synthesis of lithium-1,3-benzazaphospholides and reactivity towards organoelement and organometal halides
 AUTHOR(S): Surana, Anushka; Singh, Shreeyukta; Bansal, Raj Kumar; Peulecke, Normen; Spannenberg, Anke; Heinicke, Joachim
 CORPORATE SOURCE: Ernst-Moritz-Arndt-Universitat Greifswald, Institut fur Chemie und Biochemie, Greifswald, D-17487, Germany
 SOURCE: Journal of Organometallic Chemistry (2002), 646(1-2), 113-124
 CODEN: JORCAI; ISSN: 0022-328X
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 137:109320
 ED Entered STN: 12 Mar 2002
 AB Metalation of benzazaphospholes I (R = H, R1 = Me 1a; R = R1 = Me 1b, R = H, R1 = Ph 1c, R = H, R1 = Me3C 1d; R = Me, R1 = Ph 1e) with t-BuLi provided the ambident anions 1a-eLi in high selectivity. A crystal structure anal. of 1bLi·3THF reveals monomers and coordination of Li at N. The tungsten pentacarbonyl complexes [1][W(CO)5] (2a-e, resp.) also react preferably at N as shown by the reaction of 2a and 2d with t-BuLi. Addition at the P:C bond is a minor process in the case of 2a. Compds. 1a,cLi as well as 2dLi react with alkyl halides at P to give the corresponding 3-alkyl-1,3-benzazaphospholes or the resp. W(CO)5 complex. Even acetyl and pivaloyl chloride attack 1eLi at P affording the P-acyl derivs. II (R2 = Me 5e, CMe3 6e). Silylation can occur at N or P depending on steric and electronic effects exerted by the substituent in position 2. The different effect of 2-t-Bu groups on the steric hindrance at N and P is illustrated by the mol. geometry of 1d determined by crystal structure anal. Soft organometallic halides such as Me3SnCl, CpFe(CO)2I and CpW(CO)3Cl react with 1Li preferably at P, affording stannyl or monomer organo-transition metal derivs. The products were characterized by multinuclear NMR data of all new compds.
 CC 29-7 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 75, 78
 ST benzazaphosphole lithiation; benzazaphospholide lithium prepn substitution alkylation acylation silylation; organometallic soft electrophile reaction lithium benzazaphospholide; crystal structure benzazaphospholide lithium THF prepn; mol structure benzazaphospholide lithium THF; tungsten pentacarbonyl complex lithium benzazaphospholide prepn reactivity
 IT Lithiation
 (of benzazaphospholes)
 IT Crystal structure
 Molecular structure
 (of lithiated benzazaphospholide THF complex)
 IT Acylation
 (of lithiated benzazaphospholides)
 IT Substitution reaction
 (of lithiated benzazaphospholides and their tungsten pentacarbonyl complexes)
 IT Substituent effects
 (on silylation of lithiated benzazaphospholides)
 IT 3282-30-2, Pivaloyl chloride
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (acylation by, of lithiated benzazaphospholide)
 IT 112204-64-5

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(crystal structure; lithiation and subsequent reactions with
electrophiles)
IT 442692-44-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation and subsequent reactions of)
IT 67405-19-0 67405-20-3 404578-27-4 404578-29-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation and subsequent reactions with
electrophiles)
IT 442692-40-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(preparation and methylation or reaction with soft organometallic
electrophile)
IT 1066-45-1, Chloro(trimethyl)stannane 12107-04-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with lithiated benzazaphospholide)
IT 12078-28-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with lithiated benzazaphospholides)
IT 442692-40-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(preparation and methylation or reaction with soft organometallic
electrophile)
RN 442692-40-2 HCAPLUS
CN Lithium, [2-(1,1-dimethylethyl)-1H-1,3-benzazaphospholato-κN1][1,1'-
oxybis[ethane]]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 23 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 24
ACCESSION NUMBER: 2001:749767 HCAPLUS
DOCUMENT NUMBER: 136:69855
TITLE: Direct C-3 lithiation of 1-(triisopropylsilyl)indole
AUTHOR(S): Matsuzono, M.; Fukuda, T.; Iwao, M.
CORPORATE SOURCE: Faculty of Engineering, Department of Applied
Chemistry, Nagasaki University, Nagasaki, 852-8521,
Japan
SOURCE: Tetrahedron Letters (2001), 42(43),
7621-7623
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:69855
ED Entered STN: 15 Oct 2001
AB 1-(Triisopropylsilyl)indole can be directly lithiated at 3-position with
tert-BuLi-TMEDA in hexane at 0°C for 3 h. The generated lithio
species is reacted with a variety of electrophiles to give

3-substituted 1-(triisopropylsilyl)indoles in good yields. Thus, lithiation of 1-(triisopropylsilyl)indole with tert-BuLi-TMEDA in hexane at 0°C for 3 h followed by treatment with Me₃SiCl gave 84% 3-(trimethylsilyl)-1-(triisopropylsilyl)indole.

CC 29-6 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 27

ST lithiation isopropylsilyl indole; lithiated triisopropylsilyl indole formation reaction electrophile

IT Lithiation

(of (triisopropylsilyl)indole with tert-butyllithium in presence of TMEDA)

IT Electrophiles

(reaction with lithiated (triisopropylsilyl)indole)

IT 123191-00-4, 1-(Triisopropylsilyl)indole

RL: RCT (Reactant); RACT (Reactant or reagent)

(direct lithiation with tert-butyllithium in TMEDA and sequential reaction with electrophiles)

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 24 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 25

ACCESSION NUMBER: 2001:94741 HCAPLUS

DOCUMENT NUMBER: 134:295717

TITLE: First regioselective C-2 lithiation of 3- and 4-chloropyridines

AUTHOR(S): Choppin, Sabine; Gros, Philippe; Fort, Yves

CORPORATE SOURCE: Synthese Organique et Reactivite, UMR CNRS-UHP 7565, Faculte des Sciences, Universite Henri Poincare Nancy I, Vandoeuvre-Les-Nancy, 54506, Fr.

SOURCE: European Journal of Organic Chemistry (2001), (3), 603-606

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:295717

ED Entered STN: 08 Feb 2001

AB Butyllithium and 2-(dimethylamino)ethanol together promote the clean and regioselective C2 lithiation of 3- and 4-chloropyridines, while other reagents such as LDA or BuLi/TMEDA lead to classical ortho lithiation products or mixts. of regioisomers. The method was successfully applied to the preparation of various reactive 2,3- and 2,4-disubstituted pyridines. E.g., a solution containing 3 equivalent 2-(dimethylamino)ethanol (relative to 3-chloropyridine) in hexane was treated with 6 equivalent of BuLi at -5° and stirred for 30 min.; the solution was cooled to -60° and a solution of 3-chloropyridine in hexane was added dropwise and stirred for 1 h; 4 equivalent of di-Me disulfide in hexane was added and the mixture warmed to room temperature over 1 h to give, after workup, 2-(methylthio)-3-chloropyridine in 83% isolated yield.

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

IT Regiochemistry

(preparation of disubstituted chloropyridine derivs. by regioselective lithiation of chloropyridines with butyllithium and dimethylaminoethanol followed by substitution with electrophiles)

IT Lithiation

(regioselective; preparation of disubstituted chloropyridine derivs. by regioselective lithiation of chloropyridines with butyllithium and dimethylaminoethanol followed by substitution with

- electrophiles)**
- IT 110-18-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(less optimal additive in the preparation of disubstituted chloropyridine derivs. by regioselective lithiation of chloropyridines followed by substitution with **electrophiles**)
- IT 4111-54-0, Lithium diisopropylamide
RL: RCT (Reactant); RACT (Reactant or reagent)
(less optimal base in the preparation of disubstituted chloropyridine derivs. by regioselective lithiation of chloropyridines followed by substitution with **electrophiles**)
- IT 40273-59-4P
RL: BYP (Byproduct); PREP (Preparation)
(preparation of disubstituted chloropyridine derivs. by regioselective lithiation of chloropyridines with butyllithium and dimethylaminoethanol followed by substitution with **electrophiles**)
- IT 108-01-0, 2-(Dimethylamino)ethanol 109-72-8, Butyllithium, reactions 611-74-5, N,N-Dimethylbenzamide 626-60-8, 3-Chloropyridine 626-61-9, 4-Chloropyridine 630-19-3, Pivalaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of disubstituted chloropyridine derivs. by regioselective lithiation of chloropyridines with butyllithium and dimethylaminoethanol followed by substitution with **electrophiles**)
- IT 2402-77-9P, 2,3-Dichloropyridine 14265-58-8P 22918-01-0P 22918-03-2P 26452-80-2P, 2,4-Dichloropyridine 77332-78-6P 77332-85-5P 77332-89-9P 79698-47-8P 96424-68-9P 98626-97-2P 139585-50-5P 180748-36-1P 206437-85-6P 334542-38-0P 334542-42-6P 334542-44-8P 334542-45-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of disubstituted chloropyridine derivs. by regioselective lithiation of chloropyridines with butyllithium and dimethylaminoethanol followed by substitution with **electrophiles**)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 25 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 26

ACCESSION NUMBER: 2001:303092 HCAPLUS

DOCUMENT NUMBER: 137:232164

TITLE: Unusual cleavage of the enol silane C-O bond: transformation of 2-silyloxy-1,3-diene into 1,3-dienyl-2-zirconium compounds and their cross-coupling reactions. [Erratum to document cited in CA134:265886]

AUTHOR(S): Ganchequi, Benjamin; Bertus, Philippe; Szymoniak, Jan
CORPORATE SOURCE: Reactions Selectives et Applications, CNRS and Universite de Reims, Reims, 51687, Fr.

SOURCE: Synlett (2001), (4), 564
CODEN: SYNLES; ISSN: 0936-5214

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 29 Apr 2001

AB The corrected graphical abstract is given.

CC 21-2 (General Organic Chemistry)

ST erratum enol silyl ether zirconocene carbon oxygen bond cleavage; enol silyl ether zirconocene carbon oxygen bond cleavage erratum; methylenepropenylzirconium **electrophile** substitution erratum;

dienylzirconium cross coupling erratum

IT **Cross-coupling reaction**

(preparation of siloxy-diene-derived dienyl-zirconiums by carbon-oxygen bond cleavage of enol silyl ether and their cross-coupling reaction (Erratum))

L146 ANSWER 26 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 27

ACCESSION NUMBER: 2001:646325 HCAPLUS

DOCUMENT NUMBER: 135:371820

TITLE: Synthesis, characterization, and properties of some cyclopentadienyl molybdenum nitrosyl benzyl complexes

AUTHOR(S): Legzdins, Peter; Smith, Kevin M.; Rettig, Steven J.

CORPORATE SOURCE: Dep. Chem., Univ. British Columbia, Vancouver, V6T 1Z1, Can.

SOURCE: Canadian Journal of Chemistry (2001), 79(5/6), 502-509

CODEN: CJCHAG; ISSN: 0008-4042

PUBLISHER: National Research Council of Canada

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:371820

ED Entered STN: 05 Sep 2001

AB Reaction of CpMo(NO)(CH₂Ph)Cl with Me₂Mg, Ph₂Mg, or PhCClLi reagents in THF affords the corresponding alkyl, aryl, or alkynyl CpMo(NO)(CH₂Ph)R (R = hydrocarbyl) complexes as orange powders in good yields. Unlike related 16-electron CpMo(NO)R₂ complexes, these 18-electron species exhibit good thermal stability due to their η²-benzyl-Mo interactions. Treatment of CpMo(NO)(CH₂Ph)Cl with Na(DME)Cp provides dark green Cp₂Mo(NO)(CH₂Ph), whose solid-state mol. structure was established by a single-crystal x-ray crystallog. anal. The two Cp rings display different binding modes to the Mo atom, while the benzyl ligand is coordinated to the metal center in an η¹ fashion. The triflate complex, CpMo(NO)(CH₂Ph)(OTf), was obtained by addition of AgOTf to the benzyl chloride precursor. The covalent Mo-OTf bond in this compound can be disrupted by the addition of Lewis bases (L) such as PPh₃ or pyridine, leading to the corresponding [CpMo(NO)(CH₂Ph)(L)] [OTf] have not yet been successful.

CC 29-11 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 75

IT **Coupling reaction**

(of alkyllithium and Grignard reagents with (benzyl)(chloro)(cyclopentadienyl)(nitrosyl)molybdenum)

IT 374635-61-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and attempted deprotonation of)

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 27 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 28

ACCESSION NUMBER: 2001:61278 HCAPLUS

DOCUMENT NUMBER: 134:265886

TITLE: Unusual cleavage of the enol silane C-O bond: transformation of 2-silyloxy-1,3-dienes into 1,3-dienyl-2-zirconium compounds and their cross-coupling reactions

AUTHOR(S): Ganchegui, Benjamin; Bertus, Philippe; Szymoniak, Jan

CORPORATE SOURCE: Reactions Selectives et Applications, CNRS and Universite de Reims, Reims, 51687, Fr.

SOURCE: Synlett (2001), (1), 123-125

CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:265886
ED Entered STN: 25 Jan 2001
AB Aryl enol silyl ethers and 2-silyloxy-1,3-dienes react with zirconocene to give alkenylzirconium, and novel 1-methylene-2-propenylzirconium compds. which can be used as 2-dienylation reagents. Thus, one-pot coupling of 4-phenyl-1,3-butadienyl-2-zirconocene with a range of **electrophiles** including aryl, alkynyl, allyl halides, bromine, iodine, and a Michael acceptor occurs regioselectively at the C(2) position in the presence of Pd or Cu catalysts.
CC 21-2 (General Organic Chemistry)
ST enol silyl ether zirconocene carbon oxygen bond cleavage; methylenepropenylzirconium **electrophile** substitution; dienylzirconium cross coupling
IT **Cross-coupling reaction**
(preparation of siloxy-diene-derived dienyl-zirconiums by **carbon-oxygen bond** cleavage of enol silyl ether and their cross-coupling reaction)
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 28 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 29
ACCESSION NUMBER: 2000:337126 HCAPLUS
DOCUMENT NUMBER: 133:135497
TITLE: Structural modification of carbohydrates via functionalized organolithium intermediates: EPC preparation of branched-chain functionalized sugars
AUTHOR(S): Soler, Tatiana; Bachki, Abderrazak; Falvello, Larry R.; Foubelo, Francisco; Yus, Miguel
CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de Ciencias, Universidad de Alicante, Alicante, 03080, Spain
SOURCE: Tetrahedron: Asymmetry (2000), 11(2), 493-517
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:135497
ED Entered STN: 21 May 2000
AB The reductive opening of epoxides, e.g. I (X = CH₂, RR1 = O), derived from D-glucose and D-fructose using lithium and a catalytic amount of 4,4'-di-tert-butylbiphenyl (DTBB) in THF at -78°C allows the formation of β -oxido organolithium derivs. which, by reaction with different **electrophiles** [H₂O, D₂O, Me₃SiCl, PhCHO, Me₂CO, Et₂CO, (CH₂)₅CO, CO₂] at the same temperature yields, after hydrolysis with water, the expected branched-chain functionalized carbohydrates, e.g. I (X = CH₂, R = OH, R1 = Me). An alternative route for compound 11, derived from the epoxide I (X = CH₂, RR1 = O), consists of the **deprotonation** of the chlorohydrin I (R = OH, R1 = Cl) followed by the same protocol of lithiation-reaction with an **electrophile**. Finally, the addition of the dianions (resulting from the DTBB-catalyzed lithiation of phthalan and isochroman) to the ketones, e.g. I (X = bond, RR1 = O), derived from D-glucose and D-fructose, allowed the stereoselective functionalization at the 3-position of the sugars, giving the corresponding diols, which can cyclize to the corresponding heterocycles, e.g. II, under Mitsunobu reaction conditions.

CC 33-3 (Carbohydrates)

IT **Lithiation**

Lithiation

(catalysts; structural modification of carbohydrates via functionalized **organolithium** intermediates in preparation of branched-chain functionalized glycosides)

IT Addition reaction

Lithiation

(structural modification of carbohydrates via functionalized **organolithium** intermediates in preparation of branched-chain functionalized glycosides)

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 29 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 30

ACCESSION NUMBER: 1999:569957 HCAPLUS

DOCUMENT NUMBER: 131:350838

TITLE: Generation of allylic and benzylic organolithium reagents from the corresponding ester, amide, carbonate, carbamate and urea derivatives

AUTHOR(S): Alonso, Emma; Guijarro, David; Martinez, Pedro; Ramon, Diego J.; Yus, Miguel

CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de Ciencias, Universidad de Alicante, Alicante, 03080, Spain

SOURCE: Tetrahedron (1999), 55(36), 11027-11038

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 131:350838

ED Entered STN: 09 Sep 1999

AB The reaction of different allylic and benzylic non-enolizable esters or amides, carbonates, carbamates, and ureas with an excess of lithium powder and a catalytic amount of naphthalene (10%) in the presence of an **electrophile** [iPrCHO, tBuCHO, PhCHO, Me₂CO, Et₂CO, (CH₂)₅CO, Ph₂CO, Me₃SiCl] in THF at different temps. (-78, -30 or 0°) leads, after hydrolysis with water, to the corresponding allylated or benzylated products.

CC 21-2 (General Organic Chemistry)

IT **Lithiation**

(in situ; preparation of allylic and benzylic compds. from in-situ **organolithium** esters and amides and carbonates and carbamates and ureas under Barbier reaction conditions)

IT 67-64-1, 2-Propanone, reactions 75-77-4, reactions 78-84-2, Isobutyral 96-22-0, 3-Pentanone 100-52-7, Benzaldehyde, reactions 108-94-1, Cyclohexanone, reactions 119-61-9, Benzophenone, reactions 590-86-3, Isopentanal

RL: RCT (Reactant); RACT (Reactant or reagent)

(**electrophile**; preparation of allylic and benzylic compds. from in-situ organolithium esters and amides and carbonates and carbamates and ureas under Barbier reaction conditions)

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 30 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 31

ACCESSION NUMBER: 1999:84978 HCAPLUS

DOCUMENT NUMBER: 130:237835

TITLE: Asymmetric Syntheses of Derivatives of β - and γ -Aryl and α -Alkyl Amino Acids Using

n-BuLi/(-)-Sparteine
AUTHOR(S): Kim, Bong Jin; Park, Yong Sun; Beak, Peter
CORPORATE SOURCE: Department of Chemistry, University of Illinois at
Urbana-Champaign, Urbana, IL, 61801, USA
SOURCE: Journal of Organic Chemistry (1999), 64(5),
1705-1708
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:237835

ED Entered STN: 10 Feb 1999

AB A lithiation-substitution sequence using BuLi/(-)-sparteine was used in the enantioselective syntheses of 4-phenyl- β -lactams, 3-phenyl- γ -lactams, and an α -alkyl amino acid. Thus, esterification-deprotection of β -amino acid I (Ar = 4-MeOC₆H₄; Boc = Me₃CO₂C), followed by cyclization with Me₃CMgCl gave β -lactam II (R = H). **Deprotonation** of II (R = H) with LDA and reaction with **electrophiles** gave substituted derivs. II (R = Et, Ac, CHPhOH). Treatment of cinnamylamine ArN(Boc)CH₂CH:CHPh (III) with BuLi/(-)-sparteine and CO₂, followed by hydrogenation and esterification gave (S)- γ -amino ester IV. Lithiation of III with BuLi/(-)-sparteine followed by ClCO₂Me, subsequent hydrogenation and Boc group removal gave enantiomeric (R)- γ -amino ester V. Both IV and V could be cyclized to the corresponding 3-phenyl- γ -butyrolactams by treatment with Me₃CMgCl and removal of the p-methoxyphenyl group with ceric ammonium nitrate. Finally, treatment of benzylamine ArN(Boc)CH₂Ar with BuLi/(-)-sparteine and Me triflate, subsequent p-methoxyphenyl group removal, oxidative cleavage, and esterification gave Boc-L-Ala-OMe.

CC 34-2 (Amino Acids, Peptides, and Proteins)

Section cross-reference(s): 27

IT **Lithiation**

(stereoselective; asym. syntheses of β - and γ -aryl and α -alkyl amino acid derivs. using **butyllithium** and sparteine)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 31 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 32

ACCESSION NUMBER: 1998:454918 HCAPLUS

DOCUMENT NUMBER: 129:175672

TITLE: Relative anion stabilities and transition state energies regarding vinylic vs. allylic **deprotonation** of cyclic vinyl ethers by **organolithium** reagents: an ab initio study

AUTHOR(S): Power, Trevor D.; Sebastian, John F.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, Miami University, Oxford, OH, 45056, USA

SOURCE: Tetrahedron (1998), 54(29), 8371-8392
CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 22 Jul 1998

AB The relative energies of allylic and vinylic anions of several vinyl ethers were determined by ab initio calcns. at the Hartree-Fock and 2nd-order Moller-Plesset perturbation theory (single point) levels using basis set 6-31++G(d,p) in an attempt at explaining exptl. results concerning allylic vs. vinylic **deprotonation**. A general trend with cyclic vinyl ethers was discovered where the stability of the allyl anion over the

vinyl anion in terms of ring size is $8 = 7 > 6 > 5 \approx 4$. In general, optimized vinyl anions exhibit a vinyl angle compression whereas optimized allyl anions exhibit an allyl angle expansion. Addnl., transition state structures were examined that invoke a pre-equilibrium complexation of Li to the electron rich vinyl ether oxygens prior to the formation of the deprotonation products. These transition states are suggestive of multi-center processes, precluding the formation of free ions during these deprotonation reactions. In many cases, the stabilization energy of the appropriate transition state is in agreement with the exptl. observed product.

CC 29-2 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22

ST transition state energy vinylic ether anion; ether vinylic allylic anion stability MO; Hartree Fock calcn deprotonation vinyl ether; MP2 calcn deprotonation vinylic allylic ether; deprotonation vinyl allylic ether organolithium MO

IT Carbanions

Ethers, properties

RL: PRP (Properties)

(allyl; an ab initio study of relative anion stabilities and transition state energies regarding vinylic vs. allylic deprotonation of cyclic vinyl ethers by organolithium reagents)

IT Anions

Deprotonation

HF MO (molecular orbital)

Molecular orbital methods

Moller-Plesset perturbation theory

Total energy

Transition state structure

(an ab initio study of relative anion stabilities and transition state energies regarding vinylic vs. allylic deprotonation of cyclic vinyl ethers by organolithium reagents)

IT Ethers, properties

RL: PRP (Properties)

(an ab initio study of relative anion stabilities and transition state energies regarding vinylic vs. allylic deprotonation of cyclic vinyl ethers by organolithium reagents)

IT Ethers, properties

RL: PRP (Properties)

(vinyl; an ab initio study of relative anion stabilities and transition state energies regarding vinylic vs. allylic deprotonation of cyclic vinyl ethers by organolithium reagents)

IT 40854-64-6 41523-67-5 60211-42-9 60211-45-2 66262-06-4
66262-07-5 70113-61-0 70113-64-3 76501-18-3 83352-72-1
100791-90-0 125081-53-0, properties 186750-40-3 186750-41-4
186750-42-5 186750-43-6 186750-44-7

186750-45-8 186848-72-6 186848-74-8 187030-82-6

211574-61-7 211574-62-8 211574-63-9 211574-64-0

211574-65-1 211574-66-2 211574-67-3 211574-68-4

211574-69-5 211574-70-8 211574-71-9

211574-72-0 211574-73-1 211574-74-2, properties

211574-75-3 211574-76-4 211574-77-5 211574-78-6

211574-79-7 211574-80-0 211574-81-1 211574-82-2 211574-83-3

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(ab initio study of relative anion stabilities regarding vinylic vs. allylic deprotonation of cyclic vinyl ethers by organolithium reagents)

IT 186750-42-5 186750-43-6 186750-44-7

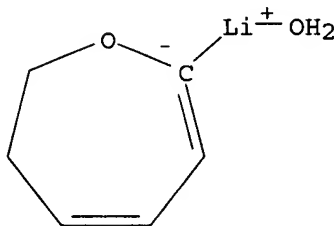
186750-45-8 211574-61-7 211574-65-1
 211574-68-4 211574-69-5 211574-70-8 21157
 4-71-9 211574-72-0 211574-73-1
 211574-77-5 211574-78-6

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(ab initio study of relative anion stabilities regarding vinylic vs. allylic deprotonation of cyclic vinyl ethers by organolithium reagents)

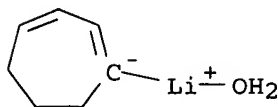
RN 186750-42-5 HCAPLUS

CN Lithium, aqua(6,7-dihydro-2-oxepinyl)- (9CI) (CA INDEX NAME)



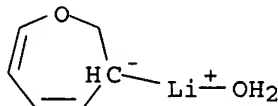
RN 186750-43-6 HCAPLUS

CN Lithium, aqua-1,3-cycloheptadien-1-yl- (9CI) (CA INDEX NAME)



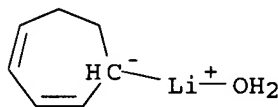
RN 186750-44-7 HCAPLUS

CN Lithium, aqua(2,3-dihydro-3-oxepinyl)- (9CI) (CA INDEX NAME)



RN 186750-45-8 HCAPLUS

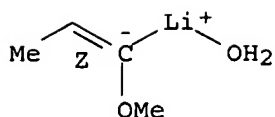
CN Lithium, aqua-2,4-cycloheptadien-1-yl- (9CI) (CA INDEX NAME)



RN 211574-61-7 HCAPLUS

CN Lithium, aqua[(1Z)-1-methoxy-1-propenyl]- (9CI) (CA INDEX NAME)

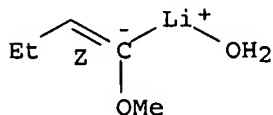
Double bond geometry as shown.



RN 211574-65-1 HCAPLUS

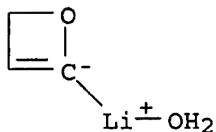
CN Lithium, aqua[(1Z)-1-methoxy-1-butenyl]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



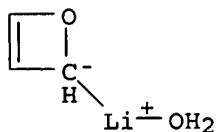
RN 211574-68-4 HCAPLUS

CN Lithium, aqua-2H-oxet-4-yl- (9CI) (CA INDEX NAME)



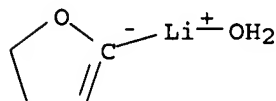
RN 211574-69-5 HCAPLUS

CN Lithium, aqua-2H-oxet-2-yl- (9CI) (CA INDEX NAME)



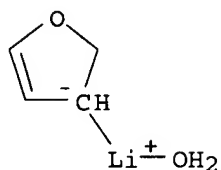
RN 211574-70-8 HCAPLUS

CN Lithium, aqua(4,5-dihydro-2-furanyl)- (9CI) (CA INDEX NAME)

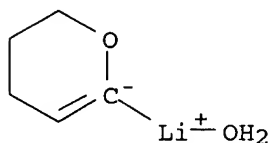


RN 211574-71-9 HCAPLUS

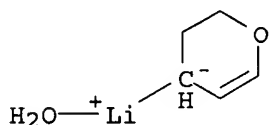
CN Lithium, aqua(2,3-dihydro-3-furanyl)- (9CI) (CA INDEX NAME)



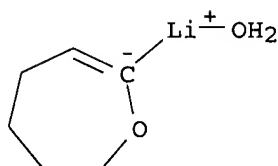
RN 211574-72-0 HCAPLUS
CN Lithium, aqua(3,4-dihydro-2H-pyran-6-yl)- (9CI) (CA INDEX NAME)



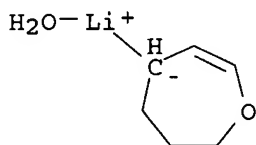
RN 211574-73-1 HCAPLUS
CN Lithium, aqua(3,4-dihydro-2H-pyran-4-yl)- (9CI) (CA INDEX NAME)



RN 211574-77-5 HCAPLUS
CN Lithium, aqua(4,5,6,7-tetrahydro-2-oxepinyl)- (9CI) (CA INDEX NAME)



RN 211574-78-6 HCAPLUS
CN Lithium, aqua(4,5,6,7-tetrahydro-4-oxepinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 32 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 33
ACCESSION NUMBER: 1998:520482 HCAPLUS
DOCUMENT NUMBER: 129:260103

TITLE: Anion translocation in organolithiums: a mechanism for the lithiation and cyclization of tertiary naphthamides

AUTHOR(S): Ahmed, Anjum; Clayden, Jonathan; Rowley, Michael

CORPORATE SOURCE: Dep. of Chemistry, University of Manchester, Manchester, M13 9PL, UK

SOURCE: Tetrahedron Letters (1998), 39(34), 6103-6106
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 21 Aug 1998

AB Deuterium labeling shows that an intramol. proton transfer ("anion translocation") is a key step in the mechanism leading to an α -lithiated tertiary naphthamide and thence to the products of anionic cyclization. The kinetic isotope effect means that proton transfer from the ortho position can become the sole mechanism for α -lithiation, though for undeuterated amides a parallel mechanism also operates in which lithiation occurs directly at the position α to nitrogen.

CC 22-12 (Physical Organic Chemistry)
Section cross-reference(s): 27, 29

IT Anions
Cyclization
Cyclization catalysts
Deprotonation
Isomerization
(anion translocation in organolithiums and mechanism for lithiation and cyclization of tertiary naphthamides)

IT Lithiation
Lithiation
(kinetics; anion translocation in organolithiums and mechanism for lithiation and cyclization of tertiary naphthamides)

IT Lithiation
(trans-; anion translocation in organolithiums and mechanism for lithiation and cyclization of tertiary naphthamides)

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 33 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 34

ACCESSION NUMBER: 1999:24332 HCAPLUS

DOCUMENT NUMBER: 130:153882

TITLE: Branched-chain functionalized carbohydrates via β -functionalized organolithium compounds

AUTHOR(S): Soler, Tatiana; Bachki, Abderrazak; Falvello, Larry R.; Foubelo, Francisco; Yus, Miguel

CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de Ciencias, Universidad de Alicante, Alicante, 03080, Spain

SOURCE: Tetrahedron: Asymmetry (1998), 9(22), 3939-3943
CODEN: TASYE3; ISSN: 0957-4166

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 13 Jan 1999

AB The reaction of an epoxysugar with an excess of lithium powder and a catalytic amount of DTBB (5 mol%) in THF at -78°C leads to the formation of the corresponding β -oxido functionalized organolithium

intermediates, which by treatment with different **electrophiles** [H₂O, D₂O, Me₃SiCl, PhCHO, Me₂CO, (CH₂)₅CO] at -78°C to room temperature affords, after hydrolysis with water, the expected enantiomerically pure compds. Starting from an epimeric epoxide and following the same procedure, using water as **electrophile**, the reduced compound was isolated, the corresponding intermediate having been involved in the process.

CC 33-3 (Carbohydrates)

IT Crystal structure

Lithiation

(preparation of branched-chain functionalized carbohydrates via functionalized **organolithium** compds.)

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 34 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 35

ACCESSION NUMBER: 1998:250350 HCAPLUS

DOCUMENT NUMBER: 129:4672

TITLE: Generation of aziridinylolithiums from sulfinylaziridines by the ligand exchange reaction of sulfoxides with tert-butyllithium: their properties and an application to asymmetric synthesis of α -dialkylamino acid ester

AUTHOR(S): Satoh, Tsuyoshi; Ozawa, Masaki; Takano, Koji; Kudo, Masabumi

CORPORATE SOURCE: Department of Chemistry, Faculty of Sciences, Science University of Tokyo, Tokyo, 162, Japan

SOURCE: Tetrahedron Letters (1998), 39(16), 2345-2348

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 129:4672

ED Entered STN: 02 May 1998

AB Aziridinylolithiums I [X = Li, R = Me, PhCH₂CH₂, Me(CH₂)₉] were generated from sulfinylaziridines [I, X = S(O)C₆H₄Me-4 (II)] by the ligand exchange reaction of the sulfoxide with tert-butyllithium. The aziridinylolithiums were stable in THF at <-30° and reacted with several **electrophiles** such as carbonyl compds. II (R = Me) reacted with t-BuLi/t-BuMgCl/THF followed by CD₃OD to give 96% yield of labeled compound I (X = D, R = Me). Optically active I (X = CO₂Et, R = Me) was prepared by the addition of (Sc,Rs)-CH₃CHClS(O)C₆H₄Me-4 to PhCH:NPh to give optically active II (R = Me) which in turn was treated with t-BuLi/t-BuMgBr and ClCO₂Et. Palladium-catalyzed hydrogenation of optically active I (X = CO₂Et, R = Me) resulted in regioselective ring cleavage to give optically active α -dialkylamino acid ester, (S)-PhNHC(CH₃)(CH₂Ph)CO₂Et.

CC 29-2 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 27

ST aziridinylolithium prepn reaction **electrophile**; sulfinylaziridine lithiation tertbutyllithium; asym synthesis alkylamino acid ester

IT **Lithiation**

(of sulfinylaziridines with tert-butyllithium to give aziridinylolithiums and asym. synthesis of α -dialkylamino acid ester)

IT **Electrophiles**

(reactions with aziridinylolithiums)

IT 119487-86-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(sequential lithiation and reaction with electrophiles)

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 35 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 36

ACCESSION NUMBER: 1998:164506 HCAPLUS

DOCUMENT NUMBER: 128:270220

TITLE: First X-ray crystal structure and NMR spectroscopic
analysis of a lithiated 1,2-diazapentadiene

AUTHOR(S): Krol, Arndt; Frohlich, Roland; Wurthwein, Ernst-Ulrich

CORPORATE SOURCE: Inst. Org. Chem., Westfalische Wilhelms-Univ.,
Munster, D-48149, GermanySOURCE: Chemical Communications (Cambridge) (1998),
(4), 485-486

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 128:270220

ED Entered STN: 20 Mar 1998

AB Deprotonation of 1,2-diazapentadienes in Et₂O leads to the resp.
lithium compds. which, in the case of [(η¹-
PhNLiNCHCMeCHPh)·Et₂O]₃, consists of an almost planar (Li-N)₃
hexagon resulting in a tunnel-like arrangement of the W-shaped
1,2-diazapentadienyl chains; the X-ray structure, solution NMR spectra and
reactions with electrophiles are reported.

CC 22-3 (Physical Organic Chemistry)

Section cross-reference(s): 29, 75

IT Conformation

Conjugation (bond)

Crystal structure

Deprotonation

Electron delocalization

Electron density

Electrophiles

Internal rotation

Lithiation

MP2 (Moller-Plesset)

Molecular structure

Overhauser effect

PM3 (molecular orbital)

Proton NMR spectroscopy

RHF (molecular orbital)

Regiochemistry

Trimerization

(x-ray crystal structure and NMR spectroscopic anal. of lithiated
1,2-diazapentadiene)

IT 205581-24-4P

RL: PEP (Physical, engineering or chemical process); PRP (Properties);

RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

PROC (Process); RACT (Reactant or reagent)

(crystallog.; x-ray crystal structure and NMR spectroscopic anal. of
lithiated 1,2-diazapentadiene)

IT 205581-23-3 205581-25-5

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical
process); PRP (Properties); RCT (Reactant); FORM (Formation,
nonpreparative); PROC (Process); RACT (Reactant or reagent)

(x-ray crystal structure and NMR spectroscopic anal. of
lithiated 1,2-diazapentadiene)

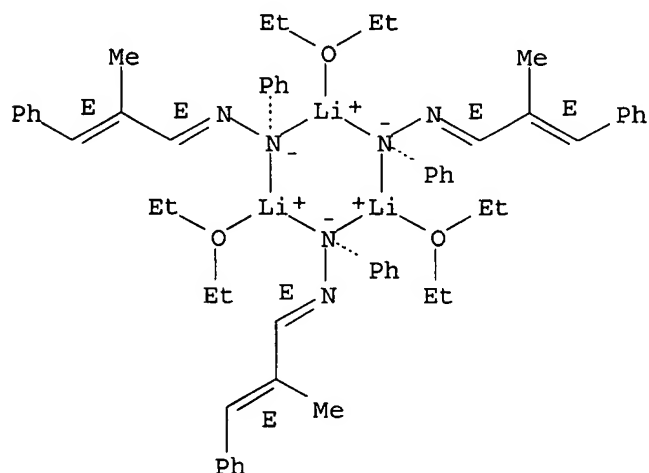
IT 205581-24-4P

RL: PEP (Physical, engineering or chemical process); PRP (Properties);
 RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 PROC (Process); RACT (Reactant or reagent)
 (crystallog.; x-ray crystal structure and NMR spectroscopic anal. of
 lithiated 1,2-diazapentadiene)

RN 205581-24-4 HCAPLUS

CN Lithium, tris[μ-(2-methyl-3-phenyl-2-propenal phenylhydrazonato-
 κN2:κN2)]tris[1,1'-oxybis[ethane]]tri-, cyclo, (all-E)- (9CI)
 (CA INDEX NAME)

Relative stereochemistry.
 Double bond geometry as shown.



IT 205581-25-5

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical
 process); PRP (Properties); RCT (Reactant); FORM (Formation,
 nonpreparative); PROC (Process); RACT (Reactant or reagent)
 (x-ray crystal structure and NMR spectroscopic anal. of
 lithiated 1,2-diazapentadiene)

RN 205581-25-5 HCAPLUS

CN Lithium, tris[μ-(2-methyl-3-phenyl-2-propenal phenylhydrazonato-
 κN2:κN2)]tris[1,1'-oxybis[ethane]]tri-, cyclo, (all-E), compd.
 with hexane (6:1) (9CI) (CA INDEX NAME)

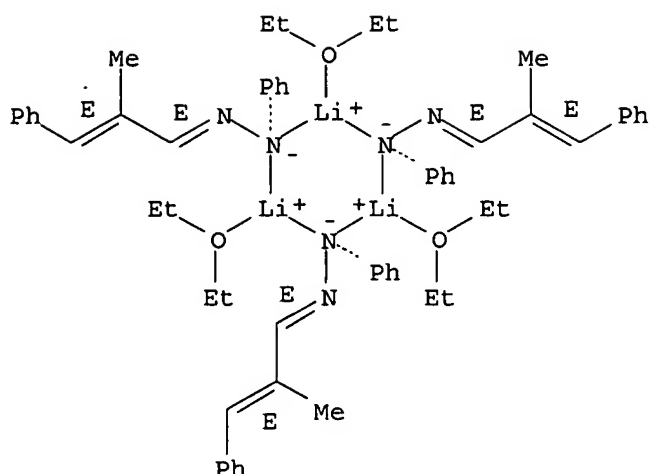
CM 1

CRN 205581-24-4

CMF C60 H75 Li3 N6 O3

CCI CCS

Relative stereochemistry.
 Double bond geometry as shown.



CM 2

CRN 110-54-3
CMF C6 H14Me-(CH₂)₄-Me

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 36 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 37

ACCESSION NUMBER: 1997:658531 HCAPLUS

DOCUMENT NUMBER: 127:318850

TITLE: Asymmetric Deprotonations: Lithiation of
N-(tert-Butoxycarbonyl)indoline with
sec-Butyllithium/(-)-SparteineAUTHOR(S): Gross, Kathleen M. Bertini; Jun, Young M.; Beak, Peter
CORPORATE SOURCE: Department of Chemistry Roger Adams Laboratory,
University of Illinois at Champaign-Urbana, Urbana,
IL, 61801, USASOURCE: Journal of Organic Chemistry (1997), 62(22),
7679-7689

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 127:318850

ED Entered STN: 17 Oct 1997

AB The asym. lithiation of N-Boc indoline with s-BuLi/(-)-sparteine and subsequent substitution provides the 2-substituted N-Boc indolines with excellent enantiomeric ratios and in variable yields. The asym. lithiation-substitution sequence with N-Boc-7-chloroindoline provides products with good enantiomeric ratios. Mechanistic investigation establishes that the enantioselectivities arise from an initial asym. deprotonation to provide the enantioenriched and configurationally stable organolithium intermediates, which react stereoselectively with electrophiles.

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 22

IT **Lithiation**

(stereoselective; of (tert-butoxycarbonyl)indolines with tert-butyllithium/(-)-sparteine)

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 37 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 38

ACCESSION NUMBER: 1997:326291 HCAPLUS

DOCUMENT NUMBER: 126:330388

TITLE: Mechanism of Lithium Diisopropylamide-Mediated Ester Deprotonation: The Role of Disolvated Monomers

AUTHOR(S): Sun, Xiufeng; Kenkre, Sarita L.; Remenar, Julius F.; Gilchrist, James H.; Collum, David B.

CORPORATE SOURCE: Department of Chemistry Baker Laboratory, Cornell University, Ithaca, NY, 14853-1301, USA

SOURCE: Journal of the American Chemical Society (1997), 119(20), 4765-4766

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 22 May 1997

AB Rate studies of lithium diisopropylamide-mediated ester metalations(I → II) are described. A fractional order dependence on the lithium diisopropylamide concentration, a first order dependence on the THF concentration, and a

substantial kinetic isotope effect reveal that the previously characterized disolvated dimers undergo deaggregation to disolvated monomers prior to a rate limiting proton transfer.

CC 22-12 (Physical Organic Chemistry)

ST lithium diisopropylamide ester deprotonation mechanism; disolvated monomer lithium diisopropylamide ester deprotonation; kinetics lithium diisopropylamide ester deprotonation

IT **Lithiation**

Lithiation

(kinetics; mechanism of lithium diisopropylamide mediated ester deprotonation)

IT Metalation kinetics

Metalation kinetics

(lithiation kinetics; mechanism of lithium diisopropylamide mediated ester deprotonation)

IT **Deprotonation**

Deprotonation kinetics

Lithiation

Proton transfer

Transition state structure

(mechanism of lithium diisopropylamide mediated ester deprotonation)

IT 7782-39-0, Deuterium, properties 7782-39-0, Deuterium, properties

RL: PRP (Properties)

(isotope effect; mechanism of lithium diisopropylamide mediated ester deprotonation)

IT 16537-05-6, tert-Butylcyclohexane carboxylate

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)

(mechanism of lithium diisopropylamide mediated ester deprotonation)

IT 141088-67-7

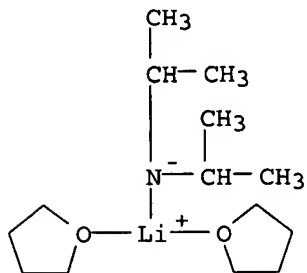
RL: RCT (Reactant); RACT (Reactant or reagent)
(mechanism of lithium diisopropylamide mediated ester
deprotonation)

IT 141088-67-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(mechanism of lithium diisopropylamide mediated ester
deprotonation)

RN 141088-67-7 HCAPLUS

CN Lithium, [N-(1-methylethyl)-2-propanaminato]bis(tetrahydrofuran) - (9CI)
(CA INDEX NAME)



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 38 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 39
ACCESSION NUMBER: 1997:198066 HCAPLUS
DOCUMENT NUMBER: 126:224873
TITLE: Pathways for Stereoinformation Transfer: Enhanced
Enantioselectivity via Diastereomeric Recycling of
Organolithium/(-)-Sparteine Complexes. [Erratum to
document cited in CA125:220905]
AUTHOR(S): Basu, Amit; Gallagher, Donald J.; Beak, Peter
CORPORATE SOURCE: Department of Chemistry, University of Illinois,
Urbana, IL, 61801, USA
SOURCE: Journal of Organic Chemistry (1997), 62(6),
1908
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 27 Mar 1997
AB The errors were not reflected in the abstract or the index entries.
CC 22-3 (Physical Organic Chemistry)
ST erratum lithiopivaloyl ethylaniline asym substitution;
lithiopivaloyl ethylaniline asym substitution erratum; kinetic resolu
electrophilic substitution erratum
IT Lithiation
Stereochemistry
Substitution reaction, electrophilic
(enhanced enantioselectivity in a lithiation-substitution sequence via
diastereomeric recycling of organolithium/(-)-sparteine
complexes (Erratum))

L146 ANSWER 39 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 40
ACCESSION NUMBER: 1997:219284 HCAPLUS
DOCUMENT NUMBER: 126:293415
TITLE: Chiral auxiliaries, ligands and arene chromium

complexes
AUTHOR(S): Kuendig, E. P.; Amurrio, D.; Anderson, G.; Beruben, D.; Khan, K.; Ripa, A.; Ronggang, L.
CORPORATE SOURCE: Dep. Chimie Organique, Univ. Geneve, Geneva, CH-1211, Switz.
SOURCE: Pure and Applied Chemistry (1997), 69(3), 543-546
CODEN: PACHAS; ISSN: 0033-4545
PUBLISHER: Blackwell
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:293415
ED Entered STN: 04 Apr 1997
AB Sequential addition of organolithium compds., RLi (R = Ph, vinyl, Me, Bu), in the presence of chiral auxiliaries, i.e., diether I, and allyl or propargyl bromide to (phenyloxazoline)Cr(CO)₃ gave 1-oxazolyl-5,6-trans-disubstituted cyclohexadienes, e.g., II,. Regioselective radical (SnBu₃) addition to the alkyne and cyclization of the vinylic radical to the diene moiety afforded fused bicyclic ring systems. Depending on whether the reaction was carried out with a terminal or internal alkyne, the reaction gave either cis-fused tetrahydroindanes or bicyclo[3.2.1]octenes selectively. Asym. methodologies for the synthesis of diastereo- or enantioenriched cyclohexadienes via temporary complexation of the arene to the **electrophilic** Cr(CO)₃ include chiral auxiliaries on the arene (oxazolines, SAMP-hydrazone), chiral ligands at Cr, chiral nucleophiles (organolithium reagents modified by chiral ligands) and planar chiral complexes synthesized via enantioselective lithiation. The article contains new developments and examples of the 1st and 3rd approach of this asym. dearomatization methodol.
CC 29-11 (Organometallic and Organometalloidal Compounds)
IT **Lithiation**
(addition of organolithium compds. and allyl- or propargyl bromide to (phenyloxazoline)chromium to give oxazolyl disubstituted cyclohexadienes)
REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L146 ANSWER 40 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 41

ACCESSION NUMBER: 1997:353854 HCAPLUS

DOCUMENT NUMBER: 127:81569

TITLE: Diastereo- and enantioselective synthesis of ferrocenylphosphines by twofold asymmetric ortho-lithiation

AUTHOR(S): Jendralla, Heiner; Paulus, Erich

CORPORATE SOURCE: Hoechst A.-G., Frankfurt/Main, D-65926, Germany

SOURCE: Synlett (1997), (5, Spec. Issue), 471-472

CODEN: SYNLES; ISSN: 0936-5214

PUBLISHER: Thieme

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 127:81569

ED Entered STN: 05 Jun 1997

AB Enantioselective **deprotonation** of diamidoferrocene I (R-R₂ = H) with BuLi/(-)-sparteine complex, followed by addition of Ph₂PCl, provided enantiomerically pure monophosphine (+)-I (R = PPh₂; R₁ = R₂ = H) after a single recrystn. When sec-BuLi/(-)-sparteine complex was employed, meso-diphosphine I (R = R₂ = PPh₂; R₁ = H) was obtained with 92% de. Conversely, treatment of homochiral I (R = PPh₂; R₁, R₂ = H) with BuLi/(-)-sparteine complex furnished enantiomerically pure C₂-sym.

diphosphine I (R = R1 = PPh2; R2 = H) with 86-94% de. Rac-I (R = PPh2; R1 = R2 = H) led in 1:1 ratio to homochiral I (R = PPh2 with R1 = PPh2, R2 = H; R1 = H, R2 = PPh2) which were characterized by x-ray structural anal.

CC 29-12 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 75

IT Lithiation

(stereoselective; preparation of ferrocenylphosphines by asym. lithiation with butyllithium in presence of sparteine)

L146 ANSWER 41 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 42

ACCESSION NUMBER: 1997:753745 HCAPLUS

DOCUMENT NUMBER: 128:115064

TITLE: Synthesis and structure of novel chiral oxazolinylferrocenes and oxazolinylferrocenylphosphine s, and their rhodium(I)-complexes

AUTHOR(S): Nishibayashi, Yoshiaki; Segawa, Kyohei; Arikawa, Yasuyoshi; Ohe, Kouichi; Hidai, Masanobu; Uemura, Sakae

CORPORATE SOURCE: Sakyo-ku, Graduate School of Engineering, Department of Energy and Hydrocarbon Chemistry, Kyoto University, Kyoto 606-01, Japan

SOURCE: Journal of Organometallic Chemistry (1997), 545-546, 381-398

CODEN: JORCAI; ISSN: 0022-328X

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 128:115064

ED Entered STN: 03 Dec 1997

AB A variety of chiral oxazolinylferrocenes were prepared from either ferrocenecarboxylic acid or cyanoferrocene and chiral β -amino alcs. Highly diastereoselective ortho-lithiation (84-99% de) of the oxazolinylferrocenes is accomplished with sec-butyllithium and the treatment of the lithiated compds. with an electrophile such as MeI, Ph₂PCl or (PhSe)₂ gives the corresponding ortho-substituted oxazolinylferrocenes. The x-ray crystal structure of (oxazolinyl)ferrocenes derivs. I [R', X = H, R = iPr, E = Ph₂P (10), PhSe; R' = H, X = Me, E = Ph₂P, R = iPr; and X = Ph₂P, E = H, R = R' = Ph (21)] were determined In connection with their usefulness as chiral ligands for Rh(I)-catalyzed asym. hydrosilylation of ketones, the square planar transition metal complexes having oxazolinylferrocenylphosphines, such as [II]BF₄ (L₂ = COD, R = R' = Ph; R = iPr, R' = H) and II [L₂ = Cl(CO), R, R' = same] were prepared by treatment of [Rh(COD)₂]BF₄ and [Rh(CO)₂Cl]₂ with 10 and 21, resp., and all structures were characterized spectroscopically and further confirmed by x-ray crystallog.

CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 75

ST crystal structure chiral oxazolinylferrocene oxazolinylferrocenylphosphine; mol structure chiral oxazolinylferrocene oxazolinylferrocenylphosphine; cyanoferrocene stereoselective cyclocondensation chiral amino alc; oxazolinylferrocene chiral prepn structure electrophile addn; ortholithiation stereoselective oxazolinylferrocene

IT Lithiation

(stereoselective; diastereoselective ortho-lithiation of the oxazolinylferrocenes with sec-butyllithium)

IT Addition reaction

(stereoselective; of electrophiles to lithiated chiral oxazolinylferrocenes)

IT 162157-02-0P 162157-03-1P 162157-04-2P 162157-05-3P 173065-68-4P
201484-45-9P 201484-51-7P 201556-00-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation and sequential **deprotonation** and reaction with
electrophile)

IT 201484-52-8P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(preparation, crystal structure and sequential **deprotonation** and
reaction with **electrophile**)

L146 ANSWER 42 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 43

ACCESSION NUMBER: 1996:457581 HCAPLUS

DOCUMENT NUMBER: 125:221912

TITLE: On the reason for opposite diastereoselectivities of
benzyl lithium compounds containing lithium amide and
lithium alkoxide functionalities

AUTHOR(S): Mueck-Lichtenfeld, Christian; Ahlbrecht, Hubertus

CORPORATE SOURCE: Inst. fuer Organische Chemie der Justus-Liebig-Univ.,
Giessen, D-35392, Germany

SOURCE: Tetrahedron (1996), 52(30), 10025-10042

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 125:221912

ED Entered STN: 02 Aug 1996

AB The carbolithiation of N-methyl-3-phenyl-prop-2-enylamine with
tert-butyllithium leads to the monomeric benzyl lithium compound,
PhCH(Li)CH(CMe₃)CH₂N(Li)CH₃ (1) in good yield. The consecutive reaction
of 1 with **electrophiles** exhibits a high anti
diastereoselectivity, opposite to what was earlier found for the O analog
PhCH(Li)CHBuCH₂OLi (3). PM3 semiempirical calcns. on the intermediates
show a preference of the anti configuration which is confirmed by ¹H NMR.
Measurements of the degree of aggregation show the dilithio compound 3 to
exist as a dimer and higher aggregates in THF. PM3 calcns. on this dimer
can explain the different diastereoselectivity.

CC 29-2 (Organometallic and Organometalloidal
Compounds)

IT Lithiation

(carbo-; of N-methylphenylpropenylamine with tert-butyllithium
leads to the monomeric benzyl lithium compds.)

IT Addition reaction

(diastereoselective addition of **electrophiles** to monomeric
benzyl lithium containing lithium amide)

IT **Electrophiles**

(diastereoselective addition to benzyl lithium compds. containing lithium
amide
and lithium alkoxide functionalities)

IT 181363-40-6P

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical
process); RCT (Reactant); SPN (Synthetic preparation); FORM (Formation,
nonpreparative); PREP (Preparation); PROC (Process); RACT (Reactant or
reagent)

(preparation, stereoselective addition with **electrophiles** and MO
calcns. of)

L146 ANSWER 43 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 44

ACCESSION NUMBER: 1996:733908 HCAPLUS

DOCUMENT NUMBER: 126:46863
TITLE: Synthesis of Hindered and Functionalized 1-CF3
Substituted Olefins via a Carbolithiation-Elimination-
Metalation Cascade
AUTHOR(S): Begue, Jean-Pierre; Bonnet-Delpon, Daniele; Bouvet,
Denis; Rock, Michael H.
CORPORATE SOURCE: Centre d'Etudes Pharmaceutiques, BIOCIS CNRS-URA 1843,
Chatenay-Malabry, F-92296, Fr.
SOURCE: Journal of Organic Chemistry (1996), 61(26),
9111-9114
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:46863

ED Entered STN: 14 Dec 1996

AB Addition of organolithium reagents R'Li (tert-BuLi, n-BuLi, PhLi) to trifluoromethyl enol ethers EtOC(RF):CHR (RF = CF3: R = Ph, CH:CHPh, p-MeOC6H4, CH2CH2Ph) and thio enol ethers EtSC(CF3):CHPh provided stereoselectively the corresponding trisubstituted fluoroalkenes I in 70-90% yields. The products could themselves react with organolithium reagents and undergo a vinyl metalation providing, after trapping with an **electrophile**, tetrasubstituted olefins in excellent yields and with stereoselectivity. This method can be applied to other fluoroalkyl enol ethers (RF = C2F5). The product, tetrasubstituted olefins, can be obtained directly from enol ether with 2 equiv of reagent through a carbolithiation-elimination-metalation cascade.

CC 23-3 (Aliphatic Compounds)

IT **Lithiation**

(vinylic metalation of 1-CF3-substituted olefins; stereoselective substitution reaction of trifluoromethyl enol ethers and thioethers with **organolithium** reagents for preparation of hindered and functionalized 1-CF3-substituted olefins)

L146 ANSWER 44 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 45

ACCESSION NUMBER: 1996:486189 HCAPLUS
DOCUMENT NUMBER: 125:220905
TITLE: Pathways for Stereoinformation Transfer: Enhanced
Enantioselectivity via Diastereomeric Recycling of
Organolithium/(-)-Sparteine Complexes
AUTHOR(S): Basu, Amit; Gallagher, Donald J.; Beak, Peter
CORPORATE SOURCE: Department of Chemistry, University of Illinois,
Urbana, IL, 61801, USA
SOURCE: Journal of Organic Chemistry (1996), 61(17),
5718-5719
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

ED Entered STN: 16 Aug 1996

AB The enantiomeric ratios for the asym. substitution of α -lithio-N-pivaloyl-o-ethylaniline are found to be dependent on the amount of the limiting **electrophilic** reagent, TMSCl. This consequence of kinetic resolution allows determination of the energy difference between nonequilibrating diastereomeric complexes of the organolithium intermediate. This result also allows the formation of products with amplified enantioselectivities by a diastereomeric recycling of the less reactive diastereomer via a temperature controlled asym. equilibration. A unique enantiodivergent **electrophilic** substitution of a common organolithium intermediate to provide two products that differ in absolute

configuration in a one-flask sequence is also a demonstrated consequence of the kinetic resolution
 CC 22-3 (Physical Organic Chemistry)
 ST lithiopivaloyl ethylaniline asym substitution; kinetic resolu
 electrophilic substitution
 IT Lithiation
 Stereochemistry
 Substitution reaction, **electrophilic**
 (enhanced enantioselectivity in a lithiation-substitution sequence via diastereomeric recycling of **organolithium**/(-)- sparteine complexes)

L146 ANSWER 45 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 46

ACCESSION NUMBER: 1994:164394 HCAPLUS

DOCUMENT NUMBER: 120:164394

TITLE: Preparation and reactivity of new β -nitrogen-functionalized vinylic organolithium compounds from secondary aliphatic allylamines

AUTHOR(S): Barluenga, Jose; Canteli, Rosa Maria; Florez, Josefa

CORPORATE SOURCE: Fac. Quim., Univ. Oviedo, Oviedo, 33071, Spain

SOURCE: Journal of Organic Chemistry (1994), 59(3), 602-6

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 120:164394

ED Entered STN: 02 Apr 1994

AB Two new types of β -nitrogen-functionalized vinylic organolithium compds. were prepared from secondary aliphatic allylamines through the temporary silylation of the amino group. The monoanionic intermediates $\text{CH}_2:\text{C}(\text{Li})\text{CH}_2\text{N}(\text{SiMe}_3)\text{R}$ 4, stable at -80° , are generated by a bromine-lithium exchange reaction. and the dianionic derivs. $\text{CH}_2:\text{C}(\text{Li})\text{CH}_2\text{N}(\text{Li})\text{R}$ 2, stable at room temperature, by a tin-lithium transmetalation reaction. Both types of organolithium compds. react with different **electrophiles** giving functionalized allylamines. Moreover, dianionic derivs. I, II can be prepared directly by bromine-lithium exchange when the β -elimination reaction of hydrogen bromide in the lithium 2-bromoallylamide is structurally hindered. Addnl., a novel type of anionic 1,3-rearrangement of a trimethylsilyl group from nitrogen to carbon is described.

CC 29-8 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 21

IT Lithiation

(of secondary aliphatic allylamines, nitrogen-functionalized vinylic **organolithium** compds. from)

IT 153476-26-7P 153476-27-8P 153476-28-9P 153476-29-0P 153476-30-3P 153476-31-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation, lithiation, and reaction of, with **electrophiles**)

L146 ANSWER 46 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 47

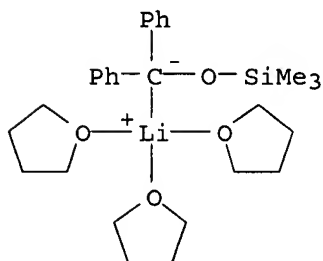
ACCESSION NUMBER: 1994:217765 HCAPLUS

DOCUMENT NUMBER: 120:217765

TITLE: α -Oxygen-substituted **organolithium** compounds and their carbenoid nature: reactions with RLi and other nucleophiles, experimental and IGLO-calculated carbon-13 NMR shifts of the carbenoid C atom

AUTHOR(S): Boche, Gernot; Bosold, Ferdinand; Lohrenz, John C. W.;
Opel, Achim; Zulauf, Peter
CORPORATE SOURCE: Fachbereich Chem., Univ. Marburg, Marburg, D-35032,
Germany
SOURCE: Chemische Berichte (1993), 126(8), 1873-85
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 30 Apr 1994
AB The authors provide evidence for the carbenoid character in α -
lithiated ethers, which was demonstrated earlier by the C-O
bond elongation between the anionic carbon atom and
oxygen. Thus, α -lithiated ethers $\text{RCH}(\text{Li})\text{OR}'$ react
as electrophiles with nucleophiles $\text{R}''\text{Li}$ to give $\text{RCH}(\text{Li})\text{R}'' +$
 LiOR' , and the ^{13}C -NMR signal of the carbenoid C atom is shifted downfield
(compared to the ^{13}C signal of the corresponding non-lithiated
compound). Since the latter two observations are also made in the
Li/halcarbenoid series, α -lithiated ethers indeed are
Li/oxygen carbenoids. Furthermore, for the first time the authors have
calculated the ^{13}C shifts of carbenoid C atoms in the Li/oxygen carbenoid
series by means of the IGLO method: the calculated data agree nicely with the
exptl. ones. They even allow the preferred bridged structure in solution to
be determined
CC 29-2 (Organometallic and Organometalloidal
Compounds)
Section cross-reference(s): 22
ST carbenoid alpha lithiated ether; NMR carbon 13 alpha
lithiated ether; IGLO alpha lithiated ether carbenoid
NMR; mol structure alpha lithiated ether IGLO
IT Electrophiles
(carbenoid α -lithiated ethers)
IT Transition state structure
(for reaction of carbenoid α -lithiated ether with
organolithium compound)
IT Molecular structure
(of carbenoid α -lithiated ethers, calcn. of)
IT Nuclear magnetic resonance
(of carbenoid α -lithiated ethers, carbon-13)
IT Ethers, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(α -lithiated carbenoid, reactions with nucleophiles)
IT Molecular orbital
(individual gage for localized orbitals, of carbenoid α -
lithiated ethers, for calcn. of carbon-13 chemical shifts)
IT 153526-44-4P 153918-33-3P
RL: PREP (Preparation)
(formation and reaction of, with nucleophiles, carbenoid
nature in)
IT 153918-34-4P 153918-36-6P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in reaction of carbenoid α -
lithiated ether with organolithium)
IT 4799-68-2P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in reaction of carbenoid α -
lithiated ether with phenyllithium)
IT 108-88-3P, Toluene, preparation
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in reaction of carbenoid α -
lithiated ethers with phenyllithium)

- IT 17498-07-6P 153526-45-5P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in reaction of α - lithiated
ether with alkyllithium)
- IT 83693-58-7P 118418-18-1P 121232-32-4P
RL: PREP (Preparation)
(formation, NMR, and reaction with nucleophiles, carbenoid
nature in)
- IT 118418-22-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation of)
- IT 14629-59-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation of, for subsequent reactions with
alkyllithiums)
- IT 271-89-6, Benzofuran
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation of, for subsequent reactions with nucleophiles)
- IT 14762-74-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(nuclear magnetic resonance, of carbenoid α - lithiated
ethers, carbon-13)
- IT 83693-60-1P 153526-38-6P 153526-39-7P 153526-40-0P 153526-41-1P
153526-42-2P 153526-43-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and lithiation of)
- IT 153918-35-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, in reaction of carbenoid α - lithiated ether
with organolithium)
- IT 153918-37-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with alkyllithiums, absence of carbenoid nature
in)
- IT 591-51-5, Phenyllithium
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with carbenoid α - lithiated ethers)
- IT 153918-37-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with alkyllithiums, absence of carbenoid nature
in)
- RN 153918-37-7 HCAPLUS
CN Lithium, [diphenyl[(trimethylsilyl)oxy]methyl]tris(tetrahydrofuran)-,
(T-4)- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1992:408060 HCAPLUS
 DOCUMENT NUMBER: 117:8060
 TITLE: Reaction between (chlorodimesitylsilyl)diarylgermanes and tert-butyllithium in THF: the formation of new germyllithium compounds
 AUTHOR(S): Baines, Kim M.; Groh, Robert J.; Joseph, Babu; Parshotam, Umesh R.
 CORPORATE SOURCE: Dep. Chem., Univ. West. Ontario, London, ON, N6A 5B7, Can.
 SOURCE: Organometallics (1992), 11(6), 2176-80
 CODEN: ORGND7; ISSN: 0276-7333
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 117:8060
 ED Entered STN: 11 Jul 1992
 AB Treatment of (chlorodimesitylsilyl)diarylgermanes [Ar = 2,4,6-trimethylphenyl (Mes), 2,4,6-triisopropylphenyl] with excess tert-butyllithium in THF followed by quenching the reaction mixture with methanol gave (dimesitylsilyl)diarylgermanes (Ar = Mes, 2,4,6-triisopropylphenyl). Surprisingly, when either reaction mixture was quenched with methanol-d₄, the corresponding (dimesitylsilyl)diaryldeuterio germanes (Ar = Mes, 2,4,6-triisopropylphenyl) were formed. The germyllithium compound Ar₂GeLiSiHMe₂ has been proposed as an intermediate. The germyllithium intermediate (Ar = Mes) was also trapped with other electrophiles, e.g. Me iodide, chlorotrimethylsilane, and benzyl bromide, to give Mes₂GeESiHMe₂ (E = Me, SiMe₃, Br). Possible mechanisms for the formation of these compds. are also discussed.
 CC 29-8 (Organometallic and Organometalloidal Compounds)
 ST germyllithium aryl prepn reaction electrophile; germanium silicon bond silylgermane; lithiation chlorodimesitylsilyldiarylgermane
 IT Lithiation
 (of (chlorodimesitylsilyl)diarylgermanes with tert-butyllithium)

L146 ANSWER 48 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 50

ACCESSION NUMBER: 1992:185028 HCAPLUS
 DOCUMENT NUMBER: 116:185028
 TITLE: Tris(phenylimido) complexes of niobium and tantalum: preparation and properties of the d⁰ [M(=NR)₃]- (M = Nb, Ta) functional group
 AUTHOR(S): Smith, David P.; Allen, Kevin D.; Carducci, Michael D.; Wigley, David E.
 CORPORATE SOURCE: Dep. Chem., Univ. Arizona, Tucson, AZ, 85721, USA
 SOURCE: Inorganic Chemistry (1992), 31(8), 1319-20
 CODEN: INOCAJ; ISSN: 0020-1669
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 03 May 1992
 AB Nb(:Nmes)2Cl(py)₂ (mes = 2,4,6-C₆H₂Me₃) is prepared from the reaction of [Nb(Net₂)2Cl₃]₂ with 2 equiv of LiNHmes per Nb. [Nb(Net₂)2Cl₃]₂ reacts with excess LiNHmes in THF to provide [Li(THF)₂]₂[Nb(:Nmes)₃(NHmes)]. Similarly, [Li(THF)₂]₂[Ta(:Nmes)₃(NHmes)] is prepared from [Ta(Net₂)2Cl₃]₂ by a parallel procedure. Expts. are presented that suggest the tris(imido) functional group [Nb(:NR)₃]- arises via an intermol. deprotonation of [Nb(:NR)₂(NHR)₂]-. [Li(THF)₂]₂(Nb(:Nmes)₃(NHmes)] reacts with 1 equiv of BuLi to form [Li(THF)₂]₂Nb(:Nmes)₃(Bu). An imprecise structure of this compound has been determined [Li(THF)₂]₂Nb(:Nmes)₃(Bu) crystallizes in the monoclinic space group, P2₁/c, with a 12.568(3), b 12.494(2), c 34.402(7) Å,

β 92.84(1)°, and $Z = 4$. The structure reveals lithium association with the imido ligands.

CC 75-7 (Crystallography and Liquid Crystals)

Section cross-reference(s): 29

IT 139606-43-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT (Reactant or reagent)

(preparation and deprotonation of)

IT 139583-05-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT (Reactant or reagent)

(preparation and reaction of, with pyridine or butyllithium)

IT 139606-43-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT (Reactant or reagent)

(preparation and deprotonation of)

RN 139606-43-2 HCAPLUS

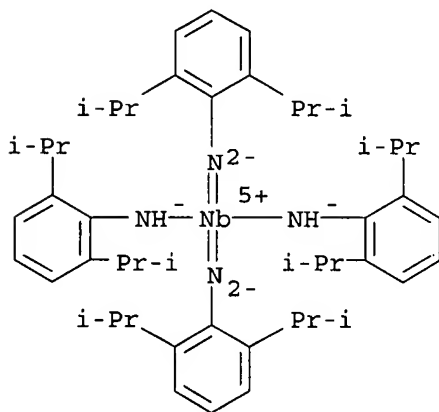
CN Lithium(1+), tetrakis(tetrahydrofuran)-, (T-4)-, (T-4)-bis[2,6-bis(1-methylethyl)benzenaminato]bis[2,6-bis(1-methylethyl)benzenaminato(2-)]niobate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 139606-42-1

CMF C48 H70 N4 Nb

CCI CCS

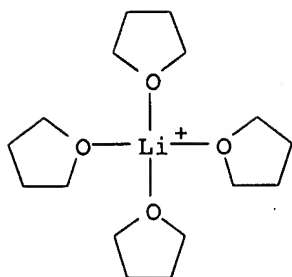


CM 2

CRN 48186-27-2

CMF C16 H32 Li O4

CCI CCS



IT 139583-05-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT (Reactant or reagent)

(preparation and reaction of, with pyridine or butyllithium)

RN 139583-05-4 HCAPLUS

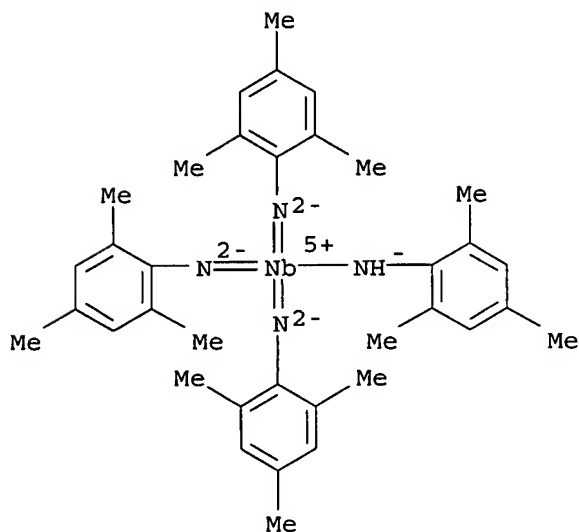
CN Lithium(1+), bis(tetrahydrofuran)-, (T-4)-(2,4,6-trimethylbenzenaminato)tris[2,4,6-trimethylbenzenaminato(2-)]niobate(2-)
(2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 139583-04-3

CMF C36 H45 N4 Nb

CCI CCS

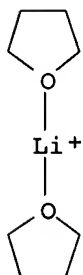


CM 2

CRN 58702-68-4

CMF C8 H16 Li O2

CCI CCS



L146 ANSWER 49 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 51
 ACCESSION NUMBER: 1993:233951 HCAPLUS
 DOCUMENT NUMBER: 118:233951
 TITLE: Studies of 2-substituted imidazoles. 3. Metalation of 1-methyl-2-phenyl- and 1-methyl-2-(2-furyl)imidazoles
 AUTHOR(S): Stojanov, V. M.; Elchaninov, M. M.; Pozharskii, A. F.
 CORPORATE SOURCE: Rostov. Gos. Univ., Rostov-on-Don, 344006, Russia
 SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1992), (1), 61-6
 CODEN: KGSSAQ; ISSN: 0132-6244
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 ED Entered STN: 12 Jun 1993
 AB Metalation of 1-methyl-2-phenylimidazole I (R = H) by BuLi gives the 5-lithiated derivative; under the same conditions 2-(2-furyl)-1-methylimidazole II (R1 = R2 = H) is metalated only at the 3-position of the furan ring. Addition of Et3N or Li 2,2,6,6-tetramethylpiperidide (III) to the reaction mixture leads only to the formation of 5-substituted furyl derivs. Thus, I and DMF, CO2, PhCHO, and PhCN gave I [R = CHO, CO2H, CH(OH)Ph, C(=O)Ph], resp.; and II (R1 = R2 = H) and BuLi, DMF in the presence of III gave a mixture containing II (R1 = CHO, R2 = H; R1 = H, R2 = CHO).
 CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
 ST metalation methylphenylimidazole furylmethylimidazole;
 electrophile substitution methylphenylimidazole
 furylmethylimidazole
 IT **Lithiation**
 (of methyl(furyl)phenylimidazole by butyllithium and subsequent reactions of)
 IT **Electrophiles**
 (reaction of, with lithiated methylphenyl- and furylmethylimidazoles)
 IT 3475-07-8, 1-Methyl-2-phenylimidazole 32902-09-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (sequential metalation by Bu lithium and reactions with **electrophiles**)

L146 ANSWER 50 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 52
 ACCESSION NUMBER: 1992:106234 HCAPLUS
 DOCUMENT NUMBER: 116:106234
 TITLE: Triazolo[4,5-d]pyrimidines. XI. Halogen-metal exchange reaction of 5-halo-3H-1,2,3-triazolo[4,5-d]pyrimidines with butyllithium
 AUTHOR(S): Tanji, Kenichi; Kato, Hiroyuki; Higashino, Takeo
 CORPORATE SOURCE: Sch. Pharm. Sci., Univ. Shizuoka, Shizuoka, 422, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1991), 39(11), 3037-40
 CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:106234
ED Entered STN: 20 Mar 1992
AB The amino group at the 5-position on the 3H-1,2,3-triazolo[4,5-d]pyrimidine I (R = H, NMePh, R1 = NH2) ring was converted into a halogen atom (iodo, Br) by treatment with isopentyl nitrite in halomethanes in satisfactory yields. I (R = H, R1 = Br, Cl) reacted with butyllithium to give butylphenyltriazolo[4,5-d]pyrimidines II by addition of butyllithium across the C7,N6-double bond. In the case of I (R = NMePh, R1 = iodo), the halogen-metal exchange reaction proceeded and the resultant 5-lithio compound reacted with **electrophiles** to give I [R1 = CH(OH)Ph, C(OH)MeCH:CH2, CMe(OH)R2, R2 = Me, Ph].
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
ST triazolopyrimidine halo prepn lithiation; **electrophilic** addn aminoiodotriazolopyrimidine benzaldehyde ketone
IT **Lithiation**
(of halotriazolopyrimidines with **butyllithium**)
IT Addition reaction
(**electrophilic**, of lithiated triazolopyrimidines with benzaldehyde and ketones)
IT 67-64-1, Acetone, reactions 78-94-4, Methyl vinyl ketone, reactions 98-86-2, Acetophenone, reactions 100-52-7, Benzaldehyde, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(**electrophilic** addition of, to lithiated triazolopyrimidine derivative)

L146 ANSWER 51 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 53
ACCESSION NUMBER: 1992:106233 HCAPLUS
DOCUMENT NUMBER: 116:106233
TITLE: Triazolo[4,5-d]pyrimidines. X. Halogen-metal exchange reaction of 7-halo-3-phenyl-3H-1,2,3-triazolo[4,5-d]pyrimidines with butyllithium
AUTHOR(S): Tanji, Kenichi; Kato, Hiroyuki; Higashino, Takeo
CORPORATE SOURCE: Sch. Pharm. Sci., Univ. Shizuoka, Shizuoka, 422, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1991), 39(11), 2793-6
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 20 Mar 1992
AB The amino group at the 7-position in 3H-1,2,3-triazolo[4,5-d]pyrimidine I (R = NH2) was converted into a halo substituent in satisfactory yields by treatment with isopentyl nitrite in CHBr3 or CH2I2. The halogen-metal exchange reaction between I (R = iodo) and butyllithium in the presence of N,N,N',N'-tetramethylethylenediamine proceeded, to give I (R = Li) which reacted smoothly with **electrophiles** leading to I [R = PhCO, PhCHOH, Me2COH, Ph2COH, MeC(OH)CH:CH2]. On the other hand, the reaction of I (R = Cl) with butyllithium gave the ring fission product, 5-amino-1-phenyl-1H-1,2,3-triazole-4-carbonitrile (II).
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
ST halogen metal exchange halophenyltriazolopyrimidine; lithiation halophenyltriazolopyrimidine; lithiophenyltriazolopyrimidine prepn addn **electrophile**; triazolopyrimidine lithiophenyl addn **electrophile**; ring cleavage chlorophenyltriazolopyrimidine butyllithium
IT **Lithiation**
(of halophenyltriazolopyrimidines with **butyllithium**)
IT Addition reaction
(of lithiophenyltriazolopyrimidine with **electrophiles**)

IT 139300-70-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, lithiation, dimerization, and protonation or reaction with
electrophiles)

L146 ANSWER 52 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 54

ACCESSION NUMBER: 1991:491997 HCAPLUS

DOCUMENT NUMBER: 115:91997

TITLE: Preparation of 1-hydroxyindole derivatives and a new
route to 2-substituted indolesAUTHOR(S): Kawasaki, Toshiya; Kodama, Atsushi; Nishida, Tokiko;
Shimizu, Kazuhisa; Somei, Masanori

CORPORATE SOURCE: Fac. Pharm. Sci., Kanazawa Univ., Kanazawa, 920, Japan

SOURCE: Heterocycles (1991), 32(2), 221-7

CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 115:91997

ED Entered STN: 06 Sep 1991

AB An easy method for the preparation and handling of 1-hydroxyindole is
developed. Based on this method, reactions of 1-hydroxyindole derivs. I
[R = Me, allyl, tosyl, Me(CH₂)₅, PhCH₂, (E)-PhCH:CHCH₂, Me₂CH:CHCH₂,
Me₃SiMe₂, Bz] are investigated. A new regioselective lithiation of
1-methoxyindole and its application for the synthesis of 2-substituted
indoles II (R₁ = CMe₂OH, CPh₂OH, 1-methyl-4-piperidiny, CHO, CO₂Me, iodo)
are also reported.

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))

ST hydroxylation dihydroindole peroxide tungstate; hydroxyindole alkylation
electrophile; lithiation methoxyindole regiochem; indole
substituted

IT Lithiation

(regioselective, of methoxyindole with butyllithium)

IT 3289-82-5P, 1-Hydroxyindole

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reactions of, with electrophiles)

L146 ANSWER 53 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 55

ACCESSION NUMBER: 1990:532252 HCAPLUS

DOCUMENT NUMBER: 113:132252

TITLE: Convenient general method for the preparation of
primary alkylolithiums by lithium-iodine exchange

AUTHOR(S): Bailey, William F.; Punzalan, Eric R.

CORPORATE SOURCE: Dep. Chem., Univ. Connecticut, Storrs, CT, 06269-3060,
USASOURCE: Journal of Organic Chemistry (1990), 55(19),
5404-6

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:132252

ED Entered STN: 13 Oct 1990

AB A general procedure is described for preparing RCH₂Li (R = alkyl) by
low-temperature Li-iodine exchange between Me₃CLi and RCH₂I. Treatment of
.apprx.0.1 M RCH₂I in 3:2 volume n-pentane-Et₂O at -78° with 2.1-2.2
equiv Me₃CLi results in clean and rapid Li-iodine exchange to generate the
corresponding RCH₂Li in virtually quant. yield. Allowing the reaction
mixture to stand at room temperature for .apprx.1 h following lithiation
removes

excess Me₃CLi via its rapid reaction with Et₂O and provides clean solns.

of RCH_2Li that may be treated with a variety of **electrophiles** to give essentially pure product in good-to-excellent yield.

CC 29-2 (Organometallic and Organometalloidal Compounds)

IT **Lithiation**

(of primary alkyl iodides with **tert-butyllithium**)

IT 542-69-8, 1-Iodobutane 629-27-6, 1-Iodooctane 629-93-6,
1-Iodooctadecane 15501-33-4, Neopentyl iodide 17376-04-4, Phenethyl
iodide 27935-87-1 51849-10-6, 1-(Iodomethyl)adamantane 79148-55-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation of, with **tert-butyllithium**, and reaction with
electrophile)

L146 ANSWER 54 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 56

ACCESSION NUMBER: 1991:122529 HCAPLUS

DOCUMENT NUMBER: 114:122529

TITLE: The directed ortho-lithiation of aryl
tetramethylphosphorodiamidates

AUTHOR(S): Watanabe, Mitsuaki; Date, Mutsuhiro; Kawanishi, Kenji;
Hori, Takako; Furukawa, Sunao

CORPORATE SOURCE: Cent. Instrum. Anal., Nagasaki Univ., Nagasaki, 852,
Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1990),
38(10), 2637-43

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:122529

ED Entered STN: 06 Apr 1991

AB Aryl tetramethylphosphorodiamidates were effectively o-lithiated with
sec-BuLi in THF at -105° . The resulting lithiated species were
trapped with a variety of **electrophiles** at -105° to
provide o-substituted phosphorodiamidates. When the lithiation was
carried out at -78° , O \rightarrow C migration of the
bis(dimethylamino)phosphoryl group took place rapidly and
2-hydroxyarylphosphonic tetramethyldiamides were produced
regioselectively. The o-directing ability of the phosphorodiamidates were
investigated by intermol. competition expts. with other directed
metalation groups.

CC 29-7 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 25

IT **Lithiation**

(ortho-, of aryl tetramethylphosphorodiamidates with sec-
butyllithium)

L146 ANSWER 55 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 57

ACCESSION NUMBER: 1990:98454 HCAPLUS

DOCUMENT NUMBER: 112:98454

TITLE: A highly convergent synthesis of
benzimidazolylpiperidines

AUTHOR(S): Carr, Albert A.; Hay, David A.; Kane, John M.;
Staeger, Michael A.

CORPORATE SOURCE: Merrell Dow Res. Inst., Cincinnati, OH, 45215, USA

SOURCE: Journal of Organic Chemistry (1990), 55(4),
1399-401

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 112:98454

ED Entered STN: 18 Mar 1990
AB Reaction of 1-[(4-fluorophenyl)methyl]-1H-benzimidazole with BuLi in THF at -78° resulted in the C2-**deprotonation** of the benzimidazole ring with no observable benzylic metalation. Reaction of this carbanion with several N-substituted piperidine-4-carboxylic acid esters afforded the corresponding benzimidazoylpiperidines I [R = H, CO₂Me₃, CH₂CH₂C₆H₄OMe-4, (CH₂)₃COC₆H₄Me₃-4].
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
IT **Lithiation**
(regioselective, of (fluorobenzyl)benzimidazole with **butyllithium**)
IT 51-17-2, Benzimidazole
RL: RCT (Reactant); RACT (Reactant or reagent)
(**deprotonation** and alkylation of, with fluorobenzyl chloride)
IT 124443-67-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and sequential **deprotonation** and substitution of, with piperidinecarboxylate, regiochem. of)

L146 ANSWER 56 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 58
ACCESSION NUMBER: 1990:478245 HCAPLUS
DOCUMENT NUMBER: 113:78245
TITLE: Methoxyethoxymethyl, tert-butoxymethyl, and benzyloxymethyl substituents as 1-protecting groups against organolithium reagents in the syntheses of imidazoles
AUTHOR(S): Ngochindo, Raphael I.
CORPORATE SOURCE: Dep. Chem., Univ. Liverpool, Liverpool, L69 3BX, UK
SOURCE: Journal of Chemical Research, Synopses (1990), (2), 58-9
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:78245

ED Entered STN: 01 Sep 1990
AB Lithiation of imidazoles I (R = MeOCH₂CH₂OCH₂, Me₃COCH₂, PhCH₂OCH₂) with BuLi followed by treatment with **electrophiles** gave 2-substituted imidazoles II [R₁ = D, Me, CHO, CO₂Et, C(OH)Ph₂].
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
IT **Lithiation**
(of imidazoles, with **organolithiums**, protective groups for)
IT 49822-58-4 128475-46-7 128475-47-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(monolithiation and reaction of, with **electrophile**)

L146 ANSWER 57 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 59
ACCESSION NUMBER: 1990:55038 HCAPLUS
DOCUMENT NUMBER: 112:55038
TITLE: Copper catalyzed reductive metalation of a propargylic epoxide to an allenyl lithium reagent
AUTHOR(S): Alexakis, A.; Marek, I.; Mangeney, P.; Normant, J. F.
CORPORATE SOURCE: Lab. Chim. Organoelem., Univ. Pierre et Marie Curie, Paris, 75252, Fr.
SOURCE: Tetrahedron Letters (1989), 30(18), 2391-2
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:55038
ED Entered STN: 17 Feb 1990
AB Phenethynyl cyclohexene oxide (I) undergoes a reductive metalation by BuLi

and catalytic amount of CuBr. The resulting allenyl lithium reagent II (R = R1 = Li) reacts normally with various **electrophiles** to give allenols II (R = H, D, Me, MeS; R1 = H) in 93-100% yields.

CC 24-5 (Alicyclic Compounds)

Section cross-reference(s): 27

ST reductive lithiation propargylic epoxide stereochem; copper catalyst
reductive lithiation propargylic epoxide; allenyl lithium reaction
electrophile

IT **Lithiation**

(reductive, stereoselective, of propargylic epoxide with
butyllithium in the presence of cuprous bromide)

IT 124707-76-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(in situ preparation and reactions of, with **electrophiles**)

L146 ANSWER 58 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 60

ACCESSION NUMBER: 1989:57216 HCAPLUS

DOCUMENT NUMBER: 110:57216

TITLE: Directed lithiation of arenethiols

AUTHOR(S): Smith, Keith; Lindsay, Charles M.; Pritchard, Gareth J.

CORPORATE SOURCE: Dep. Chem., Univ. Coll. Swansea, Swansea, SA2 8PP, UK

SOURCE: Journal of the American Chemical Society (1989
) , 111(2), 665-9

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 110:57216

ED Entered STN: 17 Feb 1989

AB Benzenethiol, toluene-4-thiol, and 3,5-dimethylbenzenethiol are doubly lithiated (on sulfur and on carbon) by BuLi in tetramethylethylenediamine. C-lithiation occurs ortho to the thiol group, and subsequent treatment with **electrophiles** provides a convenient approach to ortho-substituted arenethiol derivs. The reactions with tetraisopropylthiuram disulfide provide direct access to the resp. o-phenylene trithiocarbonates. Double lithiation of 4-methoxybenzenethiol results in C-lithiation adjacent to the methoxy group rather than the thiolate residue, indicating that methoxy is a more powerfully ortho-directing substituent in this type of metalation reaction. 3-Methoxybenzenethiol is lithiated between the methoxy and thiolate groups.

CC 25-8 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT **Lithiation**

(regioselective, of arenethiols, with **butyllithium** in
tetramethylethylenediamine)

IT 106-45-6, p-Methylbenzenethiol 696-63-9, p-Methoxybenzenethiol
15570-12-4, m-Methoxybenzenethiol 38360-81-5, 3,5-Dimethylbenzenethiol

RL: RCT (Reactant); RACT (Reactant or reagent)

(regioselective lithiation and reaction of, with **electrophile**
)

IT 108-98-5, Benzenethiol, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(regioselective lithiation and reaction of, with **electrophiles**
)

L146 ANSWER 59 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 61

ACCESSION NUMBER: 1988:55466 HCAPLUS

DOCUMENT NUMBER: 108:55466

TITLE: A simple way to some ketone homoenolates

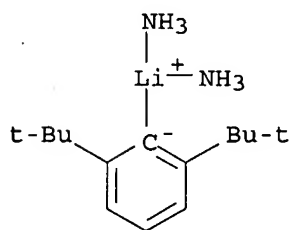
AUTHOR(S): Cuvigny, Therese; Julia, Marc; Jullien, Ludovic; Rolando, Christian
 CORPORATE SOURCE: Lab. Chim., Ec. Norm. Super., Paris, 75231/05, Fr.
 SOURCE: Tetrahedron Letters (1987), 28(23), 2587-90
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 108:55466
 ED Entered STN: 20 Feb 1988
 AB **Deprotonation** of RCH₂CH(OH)CH:CH₂ [R = Me(CH₂)₆, Me(CH₂)₉], first with K and then with BuLi, followed by quenching, gave RCH₂COEt in 70 and 77% yields, resp. Alkylation of the dianion with MeI or R₁Br [R₁ = H₂C:CHCH₂, Me(CH₂)₄, Me₂CH(CH₂)₂] gave RCH₂CO(CH₂)₂R₁, along with small amts. of RCH₂CHR₁Me, RCHR₁COEt, and dialkylated products.
 CC 23-15 (Aliphatic Compounds)
 ST ketone homoenolate alkylation regiochem; dianion allyl alc; allylic alkoxide **deprotonation** butyllithium; synthon ketone homoenolate allylic alc
 IT **Lithiation**
 (of allylic alkoxides with **butyllithium**, ketone homoenolates by)
 IT 17642-48-7, 1-Tetradecen-3-ol 51100-54-0, 1-Decen-3-ol
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (deprotonation, lithiation, hydrolysis, and alkylation of)

L146 ANSWER 60 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 62

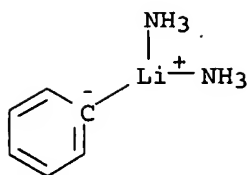
ACCESSION NUMBER: 1987:598412 HCAPLUS
 DOCUMENT NUMBER: 107:198412
 TITLE: Monomeric **organolithium** compounds in tetrahydrofuran: **tert-butyllithium**, **sec-butyllithium**, **supermesityllithium**, **mesityllithium**, and **phenyllithium**. Carbon-lithium **coupling** constants and the nature of carbon-lithium bonding
 AUTHOR(S): Bauer, Walter; Winchester, William R.; Schleyer, Paul von R.
 CORPORATE SOURCE: Inst. Org. Chem., Friedrich-Alexander Univ., Erlangen, D-8520, Fed. Rep. Ger.
 SOURCE: Organometallics (1987), 6(11), 2371-9
 CODEN: ORGND7; ISSN: 0276-7333
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 107:198412
 ED Entered STN: 27 Nov 1987
 AB Me₃CLi is a dimer in Et₂O and a monomer in THF by cryoscopy at -108° and by NMR, whereas Me₂CHCH₂Li in THF exists in a monomer-dimer equilibrium in ratios of 88:12 by cryoscopy at -108° and 78:22 by ¹³C NMR at -96°. PhLi at -103° in dilute THF is a 35:65 monomer-dimer equilibrium mixture. Addition of (Me₂NCH₂CH₂)₂NMe (PMDTA) converts all dimers to monomers. 2,4,6-R₃C₆H₂Li (R = Me₃C, Me) also are monomers. The magnitude of C-Li **coupling** consts. depends on the state of aggregation, but only to a limited extent on other factors, e.g., C hybridization, suggesting that the C-Li bond is largely ionic. The heat of **lithiation** of (Me₃C)₃C₆H₃ in an isodesmic reaction with PhLi and the effect of solvation by NH₃ on the reaction were determined by MNDO calcns.
 CC 29-2' (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 22
 ST **organolithium** aggregation THF NMR cryoscopy;

- butyllithium NMR aggregation THF; mesityllithium NMR aggregation THF; supermesityllithium NMR aggregation THF; phenyllithium NMR aggregation THF; carbon lithium coupling bond organolithium; lithium NMR butyllithium THF; dimerization organolithium THF NMR; MO dibutylbenzene lithiation isodesmic reaction
- IT Spin, nuclear coupling
(carbon-13 and lithium-6 or -7, aggregation of organolithiums in relation to)
- IT Solvation
(effect of, on heat of lithiation of dialkylbenzene with lithiobenzene)
- IT Heat of lithiation
(of dialkylbenzene with lithiobenzene, solvation by ammonia in relation to)
- IT Dimerization
(of organolithium compds. in THF, multinuclear NMR in relation to)
- IT Molecular orbital
(MNDO, of lithiation of dialkylbenzene with lithiobenzene, solvation by ammonia in relation to)
- IT Bond
(carbon-lithium, in organolithium compds., ionicity of)
- IT Nuclear magnetic resonance spectrometry
(heteronuclear double, two-dimensional, in organolithiums, of lithium-6-proton)
- IT 14258-72-1, Lithium-6, properties
RL: PRP (Properties)
(NMR of, in organolithium compds. in THF or di-Et ether)
- IT 13982-05-3, Lithium-7, properties
RL: PRP (Properties)
(NMR of, in tert-butyllithium in THF or di-Et ether)
- IT 60-29-7, Diethyl ether, properties 109-99-9, Tetrahydrofuran, properties
RL: PRP (Properties)
(aggregation of organolithium compds. in, multinuclear NMR in relation to)
- IT 594-19-4, tert-Butyllithium
RL: RCT (Reactant); RACT (Reactant or reagent)
(aggregation of, in THF and di-Et ether, multinuclear NMR and cryoscopy in relation to)
- IT 7440-44-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(bond, carbon-lithium, in organolithium compds., ionicity of)
- IT 66050-71-3 66050-73-5 110095-27-7 110095-28-8 110095-29-9 110116-26-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(carbon-13 and lithium-6 and -7 NMR coupling consts. of)
- IT 110-18-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation of, with organolithiums in THF, NMR and cryoscopy in relation to)
- IT 294-93-9, 12-Crown-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(deprotonation of, with butyllithium in THF)
- IT 598-30-1, sec-Butyllithium
RL: RCT (Reactant); RACT (Reactant or reagent)
(dimerization and complexation of, with pentamethyldiethylenetriamine in THF, cryoscopy and NMR in relation to)
- IT 110095-17-5P 110095-19-7P
RL: PREP (Preparation)

- (formation and carbon-13 NMR of, in THF)
- IT 110095-18-6P
RL: PREP (Preparation)
(formation and complexation of, with pentamethyldiethylenetriamine in THF, NMR in relation to)
- IT 110095-16-4P
RL: PREP (Preparation)
(formation and complexation of, with pentamethyldiethylenetriamine in THF, carbon-13 NMR in relation to)
- IT 110095-20-0P
RL: PREP (Preparation)
(formation and multinuclear NMR of, in di-Et ether)
- IT 71-43-2P, preparation 110095-22-2P 110095-24-4P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from lithiation of dialkylbenzene with lithiobenzene, heat of isodesmic reaction in relation to)
- IT 35383-91-6P
RL: PREP (Preparation)
(formation, MNDO calcns., and complexation of, with tetramethylethylenediamine)
- IT 591-51-5 110095-23-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation by, of dialkylbenzene, enthalpy of)
- IT 3975-77-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation of)
- IT 1014-60-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation of, with lithiobenzene, enthalpy of)
- IT 109-72-8, Butyllithium, properties
RL: PRP (Properties)
(mol. structure of, in THF and presence of chelating polyamine)
- IT 110095-24-4P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, from lithiation of dialkylbenzene with lithiobenzene, heat of isodesmic reaction in relation to)
- RN 110095-24-4 HCAPLUS
CN Lithium, diammine[2,6-bis(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)



- IT 110095-23-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation by, of dialkylbenzene, enthalpy of)
- RN 110095-23-3 HCAPLUS
CN Lithium, diamminephenyl- (9CI) (CA INDEX NAME)



L146 ANSWER 61 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 63
 ACCESSION NUMBER: 1987:617444 HCAPLUS
 DOCUMENT NUMBER: 107:217444
 TITLE: Carbon dioxide: a reagent for the simultaneous protection of nucleophilic centers and the activation of alternative locations to **electrophilic** attack. Part 8. A novel synthetic route to 4-substituted 2-pyridones
 AUTHOR(S): Katritzky, Alan R.; Fan, Wei Qiang; Koziol, Anna E.; Palenik, Gus J.
 CORPORATE SOURCE: Dep. Chem., Univ. Florida, Gainesville, FL, 32611, USA
 SOURCE: Tetrahedron (1987), 43(10), 2343-8
 CODEN: TETRAB; ISSN: 0040-4020
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 107:217444
 ED Entered STN: 12 Dec 1987
 AB **Deprotonation** of 2-pyridone (I, R = R1 = H) with BuLi, followed by carbonation with CO₂, gave lithiocarbamate I (R = CO₂Li, R1 = H). Further lithiation with Me₃CLi gave dilithio derivative I (R = CO₂Li, R1 = Li), which was quenched with a variety of **electrophiles** to give, after hydrolysis, 4-substituted pyridones I [R = H, R1 = CPh₂OH, CH(OH)C₆H₄OMe-4, CH(OH)C₆H₄Me-4, D, Me, CO₂H, CONHPh, (PH(OH)C₆H₄OMe-4, COCH₂Ph] in 49-85% yields. The regiochem. of the lithiation and addition reaction was proved by a crystal structure of I (R = H, R1 = CPh₂OH).
 CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 75
 ST lithiocarbamate protective group pyridone; lithiation
 lithiopyridonecarbamate regiochem; **electrophile** addn
 dilithiopyridonecarbamate; crystal structure pyridonyldiphenylcarbinol;
 mol structure pyridonyldiphenylcarbinol
 IT Addition reaction
 (of **electrophiles** to dilithiopyridonecarbamate, substituted
 pyridones by)
 IT **Lithiation**
 (regioselective, of lithiopyridonecarbamate, with **butyllithium**
)
 IT 142-08-5, 2-Pyridone
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (**deprotonation** of, with butyllithium)
 IT 111288-81-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reaction of, with **electrophiles**)

L146 ANSWER 62 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 64
 ACCESSION NUMBER: 1987:195901 HCAPLUS
 DOCUMENT NUMBER: 106:195901
 TITLE: The preparation and lithiation of 1-halogenocyclopropenes

AUTHOR(S): Baird, Mark S.; Hussain, Helmi H.; Nethercott, William
CORPORATE SOURCE: Dep. Org. Chem., Univ. Newcastle upon Tyne, Newcastle upon Tyne, NE1 7RU, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1986), (10), 1845-53
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 106:195901

ED Entered STN: 13 Jun 1987

AB Reaction of 1,1,2-trihalocyclopropanes (halide = Br, Cl) with MeLi in Et₂O at -90 to +20° leads to 1,2-dehalogenation to the corresponding 1-halocyclopropenes (I). I are readily lithiated by exchange with a 2nd equiv of MeLi to 1-lithiocyclopropenes, which are trapped by **electrophiles**. An exception is chlorocyclopropene II, which gives CH₂:CMeC.tplbond.CMe after Li-H exchange and LiCl loss. Cyclopropenes (X = Br, Cl) decompose to enynes or haloalkynes. A ¹²C-labeling study (sic) indicates that C-1 of the III (X = Cl) becomes C-2 of HC.tplbond.CCMe₂Cl.

CC 24-2 (Alicyclic Compounds)

IT **Lithiation**

(of halocyclopropenes with **methyllithium**)

IT Addition reaction

(nucleophilic, of lithiocyclopropenes with **electrophiles**)

L146 ANSWER 63 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 65

ACCESSION NUMBER: 1986:129216 HCAPLUS

DOCUMENT NUMBER: 104:129216

TITLE: Effect of N-butyllithium on 3-bromo-2-halopyridines (fluorine, chlorine, and bromine). Principle and study of a new reaction possibility: homotransmetalation

AUTHOR(S): Mallet, M.; Queguiner, G.

CORPORATE SOURCE: Lab. Chim. Org. Heterocycl., Inst. Natl. Super. Chim. Ind., Mont Saint Aignan, 76130, Fr.

SOURCE: Tetrahedron (1985), 41(16), 3433-40

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: French

OTHER SOURCE(S): CASREACT 104:129216

ED Entered STN: 19 Apr 1986

AB Treating 3-bromo-2-halopyridines (halo = F, Cl, Br) with BuLi involved, among other mechanisms, homotransmetalation to give the 3-lithio products. Treating the homotransmetalation products with **electrophiles**, e.g., BuBr, EtOH, pentanone, gave the 4-brominated products. The variety of products was discussed in terms of isomerization of the initial bromolithio intermediates. Thus, treating 3-bromo-2-fluoropyridine with BuLi, followed by pentanone, gave the 4-bromopyridine derivative I. On the other hand, treating 3-bromo-2-chloropyridine with BuLi, followed by pentanone, gave the pyridylpyridine derivative II.

CC 22-4 (Physical Organic Chemistry)

Section cross-reference(s): 29

IT **Lithiation**

(of bromohalopyridines by **butyllithium**, mechanism of)

L146 ANSWER 64 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 66

ACCESSION NUMBER: 1985:504657 HCAPLUS

DOCUMENT NUMBER: 103:104657

TITLE: Dilithiated synthons of tertiary benzamides, phthalamides, and O,O'-aryl dicarbamates

AUTHOR(S): Mills, R. J.; Horvath, R. F.; Sibi, M. P.; Snieckus, V.
CORPORATE SOURCE: Guelph-Waterloo Cent. Grad. Work Chem., Univ. Waterloo, Waterloo, ON, N2L 3G1, Can.
SOURCE: Tetrahedron Letters (1985), 26(9), 1145-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:104657
ED Entered STN: 04 Oct 1985
AB Benzamide I (R = Li) and phthalamide II (R1 = Li), prepared by treating I (R = Br) and II (R1 = Br) with Me3CLi, underwent reaction with **electrophiles** to afford I and II (R, R1 = D, SMe, CONEt2, iodo). In contrast to I and II, aryl dicarbamate III (R3 = H, R4 = CONEt2) underwent dilithiation directly when treated with EtMeCHLi. III (R3 = Li) reacted with **electrophiles** to give III (R3 = D, SMe, CONEt2, iodo) and underwent Fries rearrangement at room temperature to give, after treatment with K2CO3 and MeI, III (R3 = CONEt2; R4 = Me).
CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
ST lithiation bromobenzamide; phthalamide bromo lithiation; benzenediol dicarbamate lithiation; Fries rearrangement lithiated aryl dicarbamate; benzamide lithiated **electrophile** substitution; **electrophile** substitution lithiated phthalamide
IT **Lithiation**
(of diethylbenzamide, tetraethylphthalamide, and aryl dicarbamate with **alkyllithium** reagents)
IT Substitution reaction, **electrophilic**
(of dilithiated diethylbenzamide, tetraethylphthalamide, and aryl dicarbamate)
IT 97567-55-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation and reaction of, with **electrophiles**)
IT 97567-60-7P 97567-61-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of, with **electrophiles**)
IT 85370-72-5P 97567-63-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, lithiation, and reaction of, with **electrophiles**)
L146 ANSWER 65 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 67
ACCESSION NUMBER: 1983:595034 HCAPLUS
DOCUMENT NUMBER: 99:195034
TITLE: Review on the metalation of π -deficient heteroaromatic compounds. Regioselective ortho-lithiation of 3-fluoropyridine: directing effects and application to synthesis of 2,3- or 3,4-disubstituted pyridines
AUTHOR(S): Marsais, Francis; Queguiner, Guy
CORPORATE SOURCE: Lab. Chim. Org. Heterocyclique, Inst. Natl. Super. Chim. Ind. Rouen, Mont Saint Aignan, 76130, Fr.
SOURCE: Tetrahedron (1983), 39(12), 2009-21
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
OTHER SOURCE(S): CASREACT 99:195034
ED Entered STN: 12 May 1984
AB **Lithiation** of 3-fluoropyridine is chemoselective at low temps.

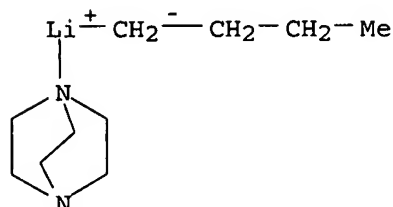
using **butyllithium**-polyamine chelates or lithium diisopropylamide. Protophilic attack by these strong bases can be directed either at the 2- or 4-position depending on the **lithiation** conditions. Various reaction parameters are studied: solvent, temperature, reaction time, lithium-chelating agent metalating agent. The high regioselectivity of 3-fluoropyridine **lithiation** is theor. discussed, in particular in terms of kinetic or thermodyn. control of the metalation. Chelation between **butyllithium** and 3-fluoropyridine is proposed, which completely modifies the heterocycle reactivity toward the **lithiating** agent. This is confirmed by theor. quantum calcns. performed on different models of 3-fluoropyridine using the CNDO/2. These results permit selection of 3-fluoropyridine metalation conditions which lead to 3-fluoro-2-lithiopyridine on the one hand and to 3-fluoro-4-lithiopyridine on the other hand. Each of the **lithiated** isomers is then reacted with a great variety of **electrophiles** to give the corresponding 2,3- or 3,4-disubstituted pyridines. Metalation of π -deficient heterocycles was also reviewed.

- CC 29-2 (Organometallic and Organometalloidal Compounds)
- ST regiochem **lithiation** fluoropyridine; pyridine fluoro **lithiation** review chem; metalation arom heterocycle
- IT Chelation
(between **butyllithium** and fluoropyridine, regiochem. of **lithiation** in relation to)
- IT Exchange reaction
(halogen-metal, between bromofluoropyridines in presence of **butyllithium**)
- IT **Lithiation**
(of fluoropyridine, regiochem. of)
- IT Regiochemistry
(of **lithiation** of fluoropyridine)
- IT Solvent effect
(on **lithiation** of fluoropyridine)
- IT Molecular orbital
(CNDO/2, of fluoropyridine, **lithiation** regiochem. in relation to)
- IT 680-31-9, uses and miscellaneous
RL: PRP (Properties)
(effect of, on **lithiation** of fluoropyridine)
- IT 87674-18-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(**formation** of aminobromopyridine from)
- IT 109-72-8P, preparation 4111-54-0 87686-24-6
RL: RCT (Reactant); RACT (**Reactant or reagent**); RACT (Reactant or reagent)
(**lithiation** by, of fluoropyridine, regiochem. of)
- IT 372-47-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(**lithiation** of, regiochem. of)
- IT 39856-58-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and **formation** of bromofluoropyridine from)
- IT 2546-52-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and halogen-metal exchange reaction of, in presence of **butyllithium**)
- IT 77332-72-0P 87674-08-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, reactions with **electrophiles**, and MO calcns. of)
- IT 87686-24-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation by, of fluoropyridine, regiochem. of)

RN 87686-24-6 HCAPLUS

CN Lithium, butyl(1,4-diazabicyclo[2.2.2]octane-N1)- (9CI) (CA INDEX NAME)



L146 ANSWER 66 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 68

ACCESSION NUMBER: 1982:472403 HCAPLUS

DOCUMENT NUMBER: 97:72403

TITLE: Preparation of functionally substituted allenes from methylacetylenes via propargylic lithium alanate or lithium borate intermediates

AUTHOR(S): Pearson, Norman R.; Hahn, Gregory; Zweifel, George
CORPORATE SOURCE: Dep. Chem., Univ. California, Davis, CA, 95616, USA
SOURCE: Journal of Organic Chemistry (1982), 47(17), 3364-6

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 97:72403

ED Entered STN: 12 May 1984

AB RC.tplbond.CMe (R = Bu, Me3C, n-C8H17, cyclohexyl) were lithiated with Me3CLi-Me2NCH2CH2NMe2, then converted into alanates or borates by reaction with (Me2CHCH2)3Al or (EtCHMe)3B. These reacted regioselectively with electrophiles (CH2:CHCH2Br, EtCHO, Me2CO, Me2C:CHCH2Br, etc.) to give 1,1-disubstituted allenes.

CC 29-2 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22, 23

ST lithium electrophile regioselective coupling; allene disubstituted

IT Coupling reaction
(of electrophiles with organolithium compds.)

IT Regiochemistry
(regioselectivity, in coupling reactions of organolithium compds. with electrophiles)

IT 82511-26-0P 82511-27-1P 82511-37-3P 82511-38-4P 82511-39-5P

82511-40-8P 82511-41-9P 82511-42-0P 82511-43-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reactions with electrophiles)

L146 ANSWER 67 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 69

ACCESSION NUMBER: 1982:34155 HCAPLUS

DOCUMENT NUMBER: 96:34155

TITLE: Nucleophilic substitutions at silicon. Evidence for ion-pair dissociation as controlling factor of the stereochemistry and a simple mechanistic proposal

AUTHOR(S): Corriu, R. J. P.; Guerin, C.

CORPORATE SOURCE: Lab. Organometall., Univ. Sci. Tech. Languedoc,

SOURCE: Montpellier, 34060, Fr.
Tetrahedron (1981), 37(14), 2467-72
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
AB The stereochem. and kinetics of the coupling reactions of chiral organosilanes with BuLi and EtLi and of their reduction with LiAlH₄ were studied. **Electrophilic** assistance to Si-X bond cleavage does not control reaction stereochem. but facilitates inversion by increasing the ability of the leaving group to depart. The dominant influence is that of ion-pair dissociation and, hence, of the electronic character of the nucleophile. A reaction mechanism is proposed, based on a description of nucleophilic substitutions at Si as a frontier-orbital process.
CC 22-4 (Physical Organic Chemistry)
IT **Coupling reaction**
(of chiral organosilanes with alkylolithiums, stereochem. and mechanism of)

L146 ANSWER 68 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 70
ACCESSION NUMBER: 1980:215240 HCAPLUS
DOCUMENT NUMBER: 92:215240
TITLE: Facile synthesis of 8-substituted quinolines
AUTHOR(S): Suggs, J. William; Pearson, G. D. N.
CORPORATE SOURCE: Bell Lab., Murray Hill, NJ, 07974, USA
SOURCE: Journal of Organic Chemistry (1980), 45(8), 1514-15
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 92:215240
ED Entered STN: 12 May 1984
AB The title compds. I (R = CDO, CHO, CHMe(OH), CH₂CH:CH₂, PPh₂, Me, SnMe₃, CH₂CH₂OH) were prepared in 32-87% yields by lithiating I (R = Br) with MeEtCHLi to give I (R = Li) followed by treatment with the appropriate **electrophile**, e.g., MeI.
CC 27-18 (Heterocyclic Compounds (One Hetero Atom))
IT **Metalation**
(lithiation, of bromoquinoline with sec-butyllithium)
IT 73038-01-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with **electrophiles**)

L146 ANSWER 69 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 71
ACCESSION NUMBER: 1980:470793 HCAPLUS
DOCUMENT NUMBER: 93:70793
TITLE: Vinyl anions. Part 8. Regioselectivity of metalation of alkylmercapto olefins
AUTHOR(S): Schmidt, Richard R.; Speer, Heike; Schmid, Bruno
CORPORATE SOURCE: Fachber. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.
SOURCE: Tetrahedron Letters (1979), (44), 4277-80
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
AB cis-EtS(O)CH:CHSEt (I) and EtSCH:CHCN underwent regioselective lithiation with Me₃CLi to give almost exclusively **α-deprotonated** vinylolithium derivs. Studies of the temperature dependence of trapping of these

derivs. with **electrophiles** showed that they are configurationally labile. I with Me₃CLi and MeOD at -100° gave 31% trans- (II) and 59% cis-EtS(O)CD:CHSet (III), and at -80° gave 73% II and 59% III.

CC 22-9 (Physical Organic Chemistry)

ST ethylsulfinylethylmercaptoethene regioselective **deprotonation** lithiation; acrylonitrile ethylmercapto regioselective **deprotonation** lithiation

IT Stereochemistry

(in **deprotonation** of ethylmercaptoethenes with tert-butyllithium)

IT Protonation and Proton transfer reaction

(**deprotonation**, of ethylmercaptoethenes with tert-butyllithium, regioselectivity in)

IT Metalation

(lithiation, of ethylmercaptoethenes with tert-butyllithium, regioselectivity in)

IT Stereochemistry

(regioselectivity, in **deprotonation** of ethylmercaptoethenes with tert-butyllithium)

IT 60036-65-9 60036-66-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(**deprotonation** of, with tert-butyllithium, regioselectivity in)

IT 74130-21-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and **deprotonation** of, with tert-butyllithium regioselectivity in)

L146 ANSWER 70 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 72

ACCESSION NUMBER: 1976:135202 HCAPLUS

DOCUMENT NUMBER: 84:135202

TITLE: Selective halogen-lithium exchange in bromophenylalkyl halides

AUTHOR(S): Parham, William E.; Jones, Lawrence D.; Sayed, Yousry A.

CORPORATE SOURCE: Paul M. Gross Chem. Lab., Duke Univ., Durham, NC, USA

SOURCE: Journal of Organic Chemistry (1976), 41(7), 1184-6

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 84:135202

ED Entered STN: 12 May 1984

AB Exchange of the aryl halide atom in o-BrC₆H₄CH₂Cl, o-BrC₆H₄(CH₂)₂Br, and o-BrC₆H₄(CH₂)₃Cl for Li was carried out with BuLi in THF-hexane at -100°. The stable lithio derivs. reacted with a variety of **electrophiles**; e.g., o-LiC₆H₄CH₂Cl (I) with H₂O, cyclohexanone, or PhNCO at low temperature gave, resp., PhCH₂Cl, II, and III. I with H₂O at room temperature gave 9,10-dihydroanthracene (not benzocyclopropene). Benzocyclobutene was formed from o-LiC₆H₄(CH₂)₂Br under similar conditions. O-halobenzyl bromides were lithiated at the benzyl bromine atom and underwent subsequent coupling to bibenzyl. O-BrC₆H₄(CH₂)₃Br with BuLi underwent intramol. coupling to indan.

CC 25-3 (Noncondensed Aromatic Compounds)

Section cross-reference(s): 26, 27

ST cyclization lithiophenylpropyl bromide; lithiophenylalkyl halide reaction **electrophile**; phenylalkyl halide lithio **electrophile**; butyllithium exchange halophenylalkyl halide; coupling benzyl bromide;

benzocyclobutene; anthracene dihydro; spirocyclohexanephthalan; phthalan
spirocyclohexane; phthalimidine phenyl

IT **Coupling reaction**
(of benzyl bromides with butyllithium)

L146 ANSWER 71 OF 115 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:885267 HCAPLUS

DOCUMENT NUMBER: 124:117147

TITLE: Chelation-directed asymmetric lithiation and
C-substitution of 1,2,4-butanetriol acetonide

AUTHOR(S): Helmke, Hendrik; Hoppe, Dieter

CORPORATE SOURCE: Organisch-Chemisches Institut, Universitaet Muenster,
Muenster, D-48149, Germany

SOURCE: Synlett (1995), (9), 978-80
CODEN: SYNLES; ISSN: 0936-5214

PUBLISHER: Thieme

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:117147

ED Entered STN: 28 Oct 1995

AB The 4-O-(2,2,4,4-tetramethyl-1,3-oxazolidine-3-carboxylate) of
(S)-1,2-O-isopropylidene-1,2,4-butanetriol is readily **deprotonated**
by sec-butyllithium in ether with high 1k-diastereoselectivity. The
presumed bicyclic chelate complex is trapped by various
electrophiles to form optically active adducts (e.g., I) with >95%
diastereoselectivity, serving as a synthetic equivalent for the unknown
(1S,3S)-1,3,4-trihydroxybutanide ion. External complexation of tertiary
diamines can compete with the internal oxygen ligand, leading to modified
stereoselectivities.

CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 22, 29

IT **Lithiation**
Stereochemistry
Synthons

(chelation-directed asym. lithiation and C-substitution of
1,2,4-butanetriol acetonide)

IT **Electrophiles**

RL: RCT (Reactant); RACT (Reactant or reagent)
(chelation-directed asym. lithiation and C-substitution of
1,2,4-butanetriol acetonide)

IT Protonation and Proton transfer reaction
(**deprotonation**, stereoselective, chelation-directed asym.
lithiation and C-substitution of 1,2,4-butanetriol acetonide)

IT Substitution reaction
(stereoselective, **electrophilic**; chelation-directed asym.
lithiation and C-substitution of 1,2,4-butanetriol acetonide)

IT 172841-63-3

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical
process); RCT (Reactant); FORM (Formation, nonpreparative); PROC
(Process); RACT (Reactant or reagent)
(chelation-directed asym. lithiation and C-substitution of
1,2,4-butanetriol acetonide)

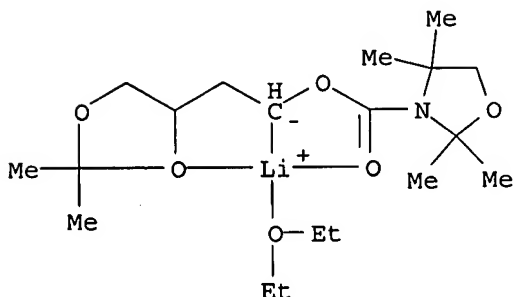
IT 172841-63-3

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical
process); RCT (Reactant); FORM (Formation, nonpreparative); PROC
(Process); RACT (Reactant or reagent)
(chelation-directed asym. lithiation and C-substitution of
1,2,4-butanetriol acetonide)

RN 172841-63-3 HCAPLUS

CN Lithium, [2-(2,2-dimethyl-1,3-dioxolan-4-yl)-1-[[2,2,4,4-tetramethyl-3-

oxazolidinyl)carbonyl]oxy]ethyl][1,1'-oxybis[ethane]]-, [T-4-[S-(R*,R*)]]-
(9CI) (CA INDEX NAME)



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L146 ANSWER 72 OF 115 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:

130:81458 CASREACT

TITLE:

The stabilization of **lithiated** organic compounds by water as a ligand. Synthesis of a new lithium-imidazole complex and regioselective reactions with selected **electrophiles**

AUTHOR(S):

Atzrodt, Jens; Beckert, Rainer; Braeuer, Michael; Nordhoff, Karsten; Anders, Ernst; Goerls, Helmar
Institut Organische Makromolekulare Chemie,
Friedrich-Schiller-Universitaet, Jena, D-07743,
Germany

CORPORATE SOURCE:

SOURCE:

European Journal of Organic Chemistry (1998
, (11), 2557-2563
CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER:

Wiley-VCH Verlag GmbH

DOCUMENT TYPE:

Journal

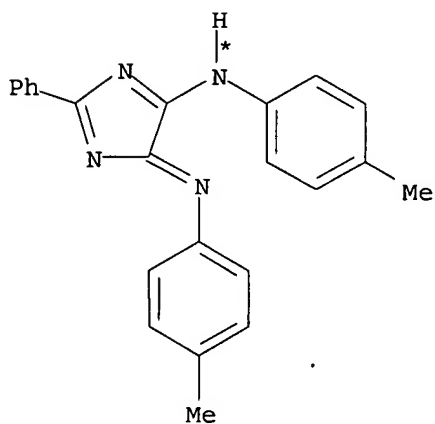
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English

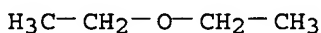
AB The **deprotonation** of the 4H-imidazoles I (R = H; R1 = 4-Me, 4-Me2N, 3-CF3) by LiH yields Li chelates which contain a stable delocalized anion. Surprisingly, the x-ray crystal structure anal. of **lithiated** I (R = H; R1 = 4-Me) reveals 1 mol. H2O in the 1st complexation sphere of Li+. This result is in good agreement with semiempirical calcns. (PM3) which predict an increase in stability on substitution of Et2O ligands by H2O mols. The **deprotonation** of I (R = H) is accompanied by a change of color from orange to purple because of the polymethinic character of the resulting anion. Alkylation as well as acylation of **lithiated** I (R = H) leads to the corresponding exocyclic substituted derivs. I (R = Me, Et, PhCH2, Ac,

PhCO). NMR of the latter and semiempirical calcns. suggest the existence of 2 rotamers due to the low rotation barrier of the exocyclic C-N bond. Another type of acylation is observed when PhCH₂COCl is used as an acylating agent. A rearrangement took place forming unsatd. amides such as imidazolylideneacetamide II.

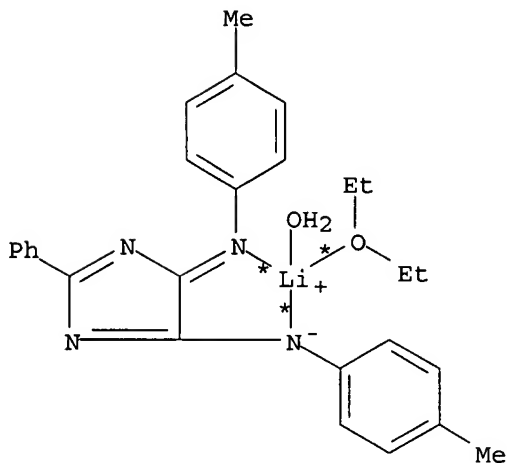
RX(4) OF 13 A + J ==> K



A



J



K

YIELD 80%

RX(4) RCT A 200510-95-8, J 60-29-7
RGT D 7580-67-8 LiH
PRO K 218966-65-5
SOL 60-29-7 Et2O

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib ab fhit 73-74

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CASREACT, USPATFULL, WPIX, MEDLINE, BIOSIS, SCISEARCH, DISSABS' - CONTINUE? (Y)/N:y

L146 ANSWER 73 OF 115 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 123:198464 CASREACT

TITLE: New one-step process for the synthesis of functionalized 1,6-dioxaspiro[4,5]decane

AUTHOR(S): Carretero, Juan C.; Rojo, Javier; Diaz, Nuria; Hamdouchi, Chafiq; Poveda, Ana

CORPORATE SOURCE: Dep. Quim. Org., Fac. Ciencias, Univ. Autonoma Madrid, Madrid, 28049, Spain

SOURCE: Tetrahedron (1995), 51(31), 8507-24
CODEN: TETRAB; ISSN: 0040-4020

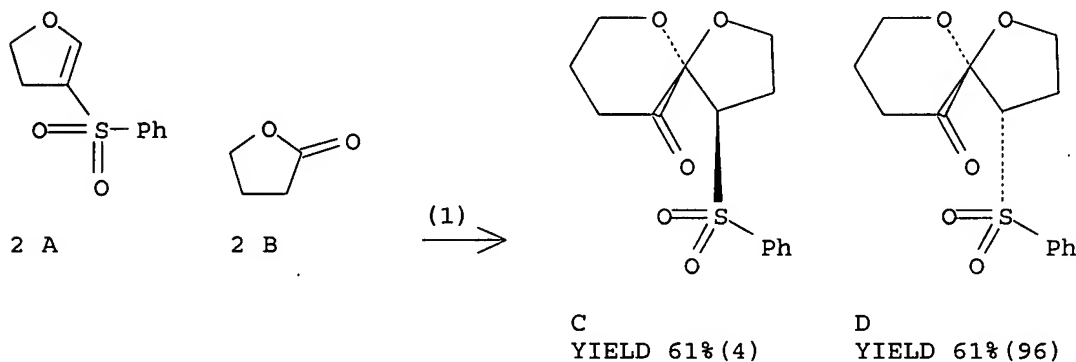
PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB β -Phenylsulfonyl dihydrofurans were readily prepared by reduction of α -phenylsulfonyl- γ -lactones with DIBAL-H, followed by dehydration with $\text{MsCl-Et}_3\text{N}$. Dihydrofurans were deprotonated with $n\text{-BuLi}$ and the resulting α -lithiated carbanion reacted with a wide variety of electrophiles. Particularly interesting is its reaction with γ -lactones which affords 1,6-dioxaspiro[4,5]decane in good yields in one-step procedure. This new method of synthesis of spiroketals, in non-acid conditions, is thermodynamically controlled and occurs with high stereoselectivity at C-4, C-5 and C-7, but not at C-2.

RX(1) OF 88 ...2 A + 2 B ==> C + D



RX(1) RCT A 133128-40-2

STAGE(1)

RGT E 109-72-8 BuLi

SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RCT B 96-48-0

STAGE(3)

RGT F 12125-02-9 NH4Cl

SOL 7732-18-5 Water

STAGE(4)

RGT G 1310-65-2 LiOH

SOL 109-99-9 THF, 7732-18-5 Water

PRO C 161113-94-6, D 161113-95-7

NTE stereoselective

L146 ANSWER 74 OF 115 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 115:136768 CASREACT

TITLE: An approach to a synthetic carboxylate-binding pocket based on β -avoparcin

AUTHOR(S): Stone, Martin J.; Van Dyk, Martha S.; Booth, Paul M.; Williams, Dudley H.

CORPORATE SOURCE: Univ. Chem. Lab., Cambridge, CB2 1EW, UK

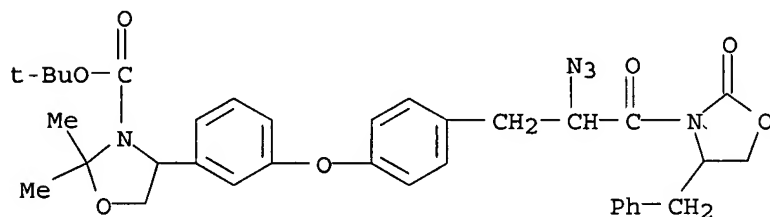
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1991), (7), 1629-35
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

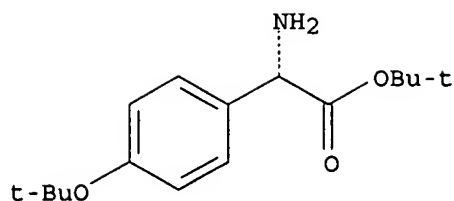
LANGUAGE: English

AB An approach to macrocyclic lactam I designed to bind to a carboxylate anion described. The diaryl ether II (R = p-C₆H₄CH:CHCO₂Me; Boc = Me₃CO₂C) was prepared by Ullmann coupling of the protected 3-hydroxyphenylglycine derivative II (R = H) and (E)-4-bromocinnamic acid Me ester. Elaboration of an optically pure (R)-tyrosine synthon was achieved by transfer of electrophilic azide to the N-acyl oxazolidinone III. The synthesis of a model system is also described.

RX(5) OF 22 ...K + P ==> Q...

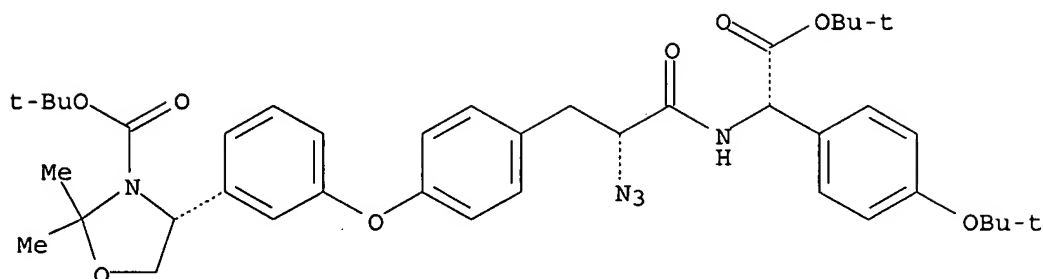


K



● HCl

(5) →

Q
YIELD 90%

RX(5) RCT K 136057-24-4

STAGE(1)

RGT R 7722-84-1 H2O2, S 1310-65-2 LiOH
SOL 109-99-9 THF, 7732-18-5 Water

STAGE(2)

RCT P 136057-26-6
RGT T 538-75-0 DCC
SOL 75-09-2 CH2Cl2

PRO Q 136057-27-7

=> d ibib ab hitstr 75-81

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CASREACT, USPATFULL, WPIX, MEDLINE, BIOSIS, SCISEARCH, DISSABS' - CONTINUE? (Y)/N:y

L146 ANSWER 75 OF 115 USPATFULL on STN DUPLICATE 5
 ACCESSION NUMBER: 2003:140951 USPATFULL
 TITLE: Silanol enzyme inhibitors
 INVENTOR(S): Sieburth, Scott McN., Coram, NY, UNITED STATES
 Mutahi, Alfred M., Edison, NJ, UNITED STATES
 Chen, Chien-An, Madison, WI, UNITED STATES

PATENT ASSIGNEE(S): Research Foundation of State University of New York
(U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2003096793	A1	20030522	<--
	US 6960678	B2	20051101	
APPLICATION INFO.:	US 2002-171560	A1	20020611	(10) <--
RELATED APPLN. INFO.:	Division of Ser. No. US 1998-194715, filed on 17 Dec 1998, GRANTED, Pat. No. US 6441212 Continuation-in-part of Ser. No. US 1996-680330, filed on 12 Jul 1996, GRANTED, Pat. No. US 5760019			
DOCUMENT TYPE:	Utility			
FILE SEGMENT:	APPLICATION			
LEGAL REPRESENTATIVE:	HOFFMANN & BARON, LLP, 6900 JERICHO TURNPIKE, SYOSSET, NY, 11791			
NUMBER OF CLAIMS:	26			
EXEMPLARY CLAIM:	1			
LINE COUNT:	1769			

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Compounds of formula (I, II or III), wherein X is OH; Y is OH, H, lower alkyl of one to six carbons or heteroatoms or F; Z and Z' are independently H, lower alkyl or Q.sub.3Si where Q is lower alkyl or aryl; n is 3-50; n' is 2-50; A and B are independently a) alkyl of one to ten carbons or heteroatoms, b) aryl of four to seven carbons or heteroatoms, c) cyclic of three to ten carbons or heteroatoms, or moieties of the formulas (d, e, or f); R.sup.1-R.sup.11 groups are each independently hydrogen, alkyl of one to ten carbons or heteroatoms, aryl of 4 to 14 carbons or heteroatoms, arylalkyl of five to twenty carbons or heteroatoms; unsubstituted carbonyl or substituted carbonyl. Heteroatoms are nitrogen, oxygen, silicon or sulfur. At least one of A or B, or both A and B are d), e), or f). The compounds of formula (I) inhibit protease enzymes and can be used as pharmaceuticals.

L146 ANSWER 76 OF 115 USPATFULL on STN

ACCESSION NUMBER: 2006:156241 USPATFULL

TITLE: Method for metal-organic production of organic intermediate products by means of aryl lithium-bases
INVENTOR(S): Meudt, Andreas, Sulzbach, GERMANY, FEDERAL REPUBLIC OF
Lehmann, Bernd, Sulzbach, GERMANY, FEDERAL REPUBLIC OF
OF
Erbes, Michael, Sulzbach, GERMANY, FEDERAL REPUBLIC OF
Forstinger, Klaus, Sulzbach, GERMANY, FEDERAL REPUBLIC OF
OF

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2006131762	A1	20060622	
APPLICATION INFO.:	US 2003-526237	A1	20030821	(10) <--
	WO 2003-EP9252		20030821	<--
			20050228	PCT 371 date

	NUMBER	DATE	
PRIORITY INFORMATION:	DE 2002-10240262	20020831	<--
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	APPLICATION		

LEGAL REPRESENTATIVE: CLARIANT CORPORATION, INTELLECTUAL PROPERTY DEPARTMENT,
4000 MONROE ROAD, CHARLOTTE, NC, 28205, US

NUMBER OF CLAIMS: 9

EXEMPLARY CLAIM: 1

LINE COUNT: 479

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention relates to a method for the production of substituted aromatic compounds by producing lithium arylene and by reacting it with suitable **electrophiles**. The method comprises the following steps (step 1); an aryl lithium compound (auxiliary base") is initially produced by reacting a halogen aromatic compound with lithium metal; said compound is subsequently (step 2) reacted for **deprotonation** of the aromatic substrate in order to form the corresponding lithium aromatic compound which is subsequently (step 3) reacted with a corresponding **electrophile** to form the desired substituted aromatic compound, see page 2 of the description.

L146 ANSWER 77 OF 115 USPATFULL on STN

ACCESSION NUMBER: 2005:296897 USPATFULL

TITLE: Method for the organometallic production of organic intermediate products comprising **carbon-heteroatom bonds** achieved by the **deprotonation of heteroatoms**

INVENTOR(S): Meudt, Andreas, Hofheim, GERMANY, FEDERAL REPUBLIC OF
Lehnemann, Bernd, Frankfurt am Main, GERMANY, FEDERAL REPUBLIC OF
Erbes, Michael, Frankfurt am Main, GERMANY, FEDERAL REPUBLIC OF
Forstinger, Klaus, Babenhausen, GERMANY, FEDERAL REPUBLIC OF

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2005258553	A1	20051124	
APPLICATION INFO.:	US 2003-526327	A1	20030821	(10) <--
	WO 2003-EP9250		20030821	
			20050228	PCT 371 date

	NUMBER	DATE	
PRIORITY INFORMATION:	DE 2002-10240260	20020831	<--
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	APPLICATION		
LEGAL REPRESENTATIVE:	CLARIANT CORPORATION, INTELLECTUAL PROPERTY DEPARTMENT, 4000 MONROE ROAD, CHARLOTTE, NC, 28205, US		
NUMBER OF CLAIMS:	8		
EXEMPLARY CLAIM:	1		
LINE COUNT:	411		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB ##STR1## ##STR2## ##STR3## The invention relates to a method for binding **heteroatom-carbon bonds**. According to said method, a lithium compound (II) is first generated by reacting aliphatic or aromatic halogen compounds (I) with lithium metal, said compound is then used for the **deprotonation** of the compounds (III) or (V). The lithium salts of formulas (IV) or (VI) obtained by said **deprotonation** are subsequently reacted with suitable **carbon electrophiles** (equation I), said process binding the **heteroatom-carbon bond** and forming the products (VIII) or (VIII), (equation I).

L146 ANSWER 78 OF 115 USPATFULL on STN
 ACCESSION NUMBER: 2002:217438 USPATFULL
 TITLE: Silanol enzyme inhibitors
 INVENTOR(S): Sieburth, Scott McN., Coram, NY, United States
 Mutahi, Alfred M., Edison, NJ, United States
 Chen, Chien-An, Madison, WI, United States
 PATENT ASSIGNEE(S): Research Foundation of State University of New York,
 Albany, NY, United States (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 6441212	B1	20020827	<--
	WO 9802578		19980122	<--
APPLICATION INFO.:	US 1998-194715		19981217 (9)	<--
	WO 1997-US12041		19970711	<--
			19981217	PCT 371 date
RELATED APPLN. INFO.:	Division of Ser. No. US 1996-680330, filed on 12 Jul 1996, now patented, Pat. No. US 5760014			
DOCUMENT TYPE:	Utility			
FILE SEGMENT:	GRANTED			
PRIMARY EXAMINER:	Low, Christopher S. F.			
ASSISTANT EXAMINER:	Lukton, David			
LEGAL REPRESENTATIVE:	Hoffmann & Baron, LLP			
NUMBER OF CLAIMS:	4			
EXEMPLARY CLAIM:	1			
NUMBER OF DRAWINGS:	0 Drawing Figure(s); 0 Drawing Page(s)			
LINE COUNT:	1543			

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Compounds of formula (I, II, or III), wherein X is OH; Y is OH, H, lower alkyl of one to six **carbons** or **heteroatoms** or F; Z and Z' are independently H, lower alkyl or Q.sub.3Si where Q is lower alkyl or aryl; n is 3-50; n' is 2-50, A and B are independently a) alkyl of one to ten **carbons** or **heteroatoms**, b) aryl of four to ten **carbons** or **heteroatoms**, c) cyclic of three to ten **carbons** or **heteroatoms**, or moieties of the formulas (d, e, or f); R.sup.1-R.sup.11 groups are each independently hydrogen, alkyl of one to ten **carbons** or **heteroatoms** aryl of 4 to 14 **carbons** or **heteroatoms**, arylalkyl of five to twenty **carbons** or **heteroatoms**; unsubstituted carbonyl or substituted carbonyl. **Heteroatoms** are **nitrogen**, **oxygen**, **silicon** or **sulfur**. At least one of A or B, or both A and B are d), e), or f). The compounds of formula (I) inhibit protease enzymes and can be used as pharmaceuticals.

L146 ANSWER 79 OF 115 USPATFULL on STN
 ACCESSION NUMBER: 2000:114136 USPATFULL
 TITLE: Synthesis of benzo[f]quinolinones
 INVENTOR(S): Brennan, John, Indianapolis, IN, United States
 Doecke, Christopher William, Indianapolis, IN, United States
 Heath, Perry Clark, Indianapolis, IN, United States
 Patterson, Lawrence Edward, Indianapolis, IN, United States
 Udodong, Uko Effiong, Indianapolis, IN, United States
 Weigel, Leland Otto, Indianapolis, IN, United States
 PATENT ASSIGNEE(S): Eli Lilly and Company, Indianapolis, IN, United States
 (U.S. corporation)

NUMBER	KIND	DATE
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PATENT INFORMATION:	US 6111110	20000829	<--
	WO 9818757	19980507	<--
APPLICATION INFO.:	US 1999-254829	19990312 (9)	<--
	WO 1997-US19229	19971027	<--
		19990312	PCT 371 date
		19990312	PCT 102(e) date

	NUMBER	DATE	
PRIORITY INFORMATION:	US 1996-27868P	19961030 (60)	<--
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	Granted		
PRIMARY EXAMINER:	Seaman, D. Margaret		
LEGAL REPRESENTATIVE:	Sayles, Michael J.		
NUMBER OF CLAIMS:	21		
EXEMPLARY CLAIM:	1		
LINE COUNT:	1339		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A process for preparing intermediates and benzoquinolin-3-one pharmaceuticals, such pharmaceuticals are effective in treating conditions consequent on 5 α -reductase.

L146 ANSWER 80 OF 115 USPATFULL on STN

ACCESSION NUMBER: 1998:61634 USPATFULL

TITLE: Silanol enzyme inhibitors

INVENTOR(S): Sieburth, Scott McN., Coram, NY, United States

Mutahi, Alfred M., Edison, NJ, United States

PATENT ASSIGNEE(S): The Research Foundation of State University of New York, Albany, NY, United States (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 5760019		19980602	<--
APPLICATION INFO.:	US 1996-680330		19960712 (8)	<--
DOCUMENT TYPE:	Utility			
FILE SEGMENT:	Granted			
PRIMARY EXAMINER:	Ketter, James			
ASSISTANT EXAMINER:	Yucel, Irem			
LEGAL REPRESENTATIVE:	Hoffman & Baron, LLP			
NUMBER OF CLAIMS:	18			
EXEMPLARY CLAIM:	1			
LINE COUNT:	1766			

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Compounds of formula I ##STR1## in which X is OH

Y is H, OH methyl or F,

A and B are independently

a) alkyl of one to ten carbons or heteroatoms,

b) aryl of four to seven carbons or heteroatoms,

c) cyclic of three to ten carbons or heteroatoms, or moieties of the formulas ##STR2## in a), b), c), d), e) and f), CH is bonded to silicon; R^{sup.1} to R^{sup.11} are independently hydrogen, alkyl of 1 to 10 carbons or heteroatoms, aryl of 4 to 14 carbons or heteroatoms, arylalkyl of 5 to 20 carbons or heteroatoms, substituted carbonyl

or unsubstituted carbonyl;

heteroatoms are nitrogen, oxygen, silicon
or sulfur; and

at least one of A and B is independently moieties d, e or f.

The compounds of formula I inhibit protease enzymes and can be used as
pharmaceuticals.

L146 ANSWER 81 OF 115 USPTF on STN
ACCESSION NUMBER: 89:74287 USPTF
TITLE: Spiro-tricyclic aromatic succinimide derivatives
INVENTOR(S): York, Jr., Billie M., Fort Worth, TX, United States
PATENT ASSIGNEE(S): Alcon Laboratories, Inc., Fort Worth, TX, United States
(U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 4864028		19890905	<--
APPLICATION INFO.:	US 1987-94636		19870909 (7)	<--
DISCLAIMER DATE:	20020827			
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 1987-5859, filed on 21 Jan 1987, now abandoned which is a continuation of Ser. No. US 1985-766569, filed on 14 Aug 1985, now abandoned which is a continuation of Ser. No. US 1983-532168, filed on 14 Sep 1983, now patented, Pat. No. US 4537892			
DOCUMENT TYPE:	Utility			
FILE SEGMENT:	Granted			
PRIMARY EXAMINER:	Schwartz, Richard A.			
LEGAL REPRESENTATIVE:	Arno, James A., Brown, Gregg C., Price, Robert L.			
NUMBER OF CLAIMS:	20			
EXEMPLARY CLAIM:	1			
LINE COUNT:	3105			
CAS INDEXING IS AVAILABLE FOR THIS PATENT.				

AB Disclosed are substituted or unsubstituted planar tricyclic fluorene or
nuclear analogs thereof, spiro-coupled to a five-membered ring
containing a secondary amide, and the pharmaceutically acceptable salts
thereof. These compounds are useful, inter alia, in the treatment of
diabetes. Also disclosed are processes for the preparation of such
compounds; pharmaceutical compositions comprising such compounds; and
methods of treatment comprising administering such compounds and
compositions when indicated for, inter alia, long term, prophylactic
treatment of the diabetes syndrome.

=> d iall abeq tech abex 82-101

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CASREACT, USPTF, WPIX, MEDLINE,
BIOSIS, SCISEARCH, DISSABS' - CONTINUE? (Y)/N:y

L146 ANSWER 82 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
ACCESSION NUMBER: 2005-304882 [31] WPIX
DOC. NO. CPI: C2005-094425
TITLE: One pot production of an organometallic compound
comprises reacting a hydrocarbon or heteroatom-containing
material with a base material, adding metal source and
reacting the hydrocarbon or heteroatom containing

compound with metal source.
 DERWENT CLASS: A85 E12 L03
 INVENTOR(S): MEIERE, S H; PETERS, D W
 PATENT ASSIGNEE(S): (MEIE-I) MEIERE S H; (PETE-I) PETERS D W; (PRAX-N)
 PRAXAIR TECHNOLOGY INC
 COUNTRY COUNT: 108
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
US 2005075510	A1	20050407	(200531)*		9	C07F001-00	
WO 2005038866	A2	20050428	(200531)	EN		H01L000-00	
RW: AT BE BG BW CH CY CZ DE DK EA EE ES FI FR GB GH GM GR HU IE IT KE							
LS LU MC MW MZ NA NL OA PL PT RO SD SE SI SK SL SZ TR TZ UG ZM ZW							
W: AE AG AL AM AT AU AZ BA BB BG BR BW BY BZ CA CH CN CO CR CU CZ DE							
DK DM DZ EC EE EG ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG							
KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NA NI NO NZ							
OM PG PH PL PT RO RU SC SD SE SG SK SL SY TJ TM TN TR TT TZ UA UG							
US UZ VC VN YU ZA ZM ZW							

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
US 2005075510	A1	US 2003-678074	20031006
WO 2005038866	A2	WO 2004-US32339	20041001

PRIORITY APPLN. INFO: US 2003-678074 20031006

INT. PATENT CLASSIF.:

MAIN: C07F001-00; H01L000-00

SECONDARY: C07F001-02

BASIC ABSTRACT:

US2005075510 A UPAB: 20050517

NOVELTY - One pot production of an organometallic compound involves reacting a hydrocarbon or heteroatom-containing material with a base material in presence of a solvent to form a first reaction mixture, adding a metal source compound to the first reaction mixture, reacting the hydrocarbon or heteroatom containing compound with the metal source compound to form a second reaction mixture of organometallic compound, followed by separation from the second reaction mixture.

DETAILED DESCRIPTION - An INDEPENDENT CLAIM is included for a one pot production of a liquid hafnium amide compound involving:

- (1) reacting an amine with a lithiated base material to produce a first reaction mixture comprising a lithium amide;
- (2) adding a hafnium halide to the first reaction mixture;
- (3) reacting the lithium amide with the hafnium halide to produce a second reaction mixture comprising the liquid hafnium amide compound; and
- (4) separating the liquid hafnium amide compound from the second reaction mixture.

USE - For the one pot production of organometallic compounds e.g. a transition metal-containing amide, alkoxide, diketone, cyclopentadienide, imide, particularly liquid hafnium amide, hafnium (IV) tert-butoxide, hafnium (IV) acetylacetonate, bis(cyclopentadienyl)hafnium dichloride and tert-butylimidobis(dimethylamino)hafnium useful for forming metal oxide films, particularly in thin film deposition.

ADVANTAGE - The method generates organometallic compound precursors that have varied chemical structures and physical properties. The method provides final products on a large scale since it can be conducted using

the same equipment, some of the same reagents and process parameters can easily be adapted to manufacture a wide range of products. The method provides for the synthesis of organometallic compounds, where all manipulations are carried out in a single vessel, and the steps do not require the isolation of an intermediate complex. The method enables the production of multi-kilogram lots of high purity organometallic compound precursors, e.g. hafnium amide.

The method produces a key, solid, raw material in-situ from liquid components. An in-line filtration or decantation step may be utilized to produce an easily distillable solution, thus minimizing exposure of moisture sensitive mixtures. The chemical vapor deposition/atomic layer deposition organometallic precursors may be utilized to form films as the first next generation high K materials to replace silicon dioxide at and/or beyond the 65 nm technology node. The overall advantage of the method is a simpler process that utilizes less expensive materials and allows for larger batch sizes. These factors translate to an economic advantage. With no loss in yield compared to prior art methods, this method avoids labor-intensive and waste generating material manipulations. The method also eliminates the formation and isolation of an intermediate, as well as reduces the amount of materials (e.g. chemical reagents, glassware) required substantially. Also, because all transformations occur in one vessel until the final product is isolated, all compounds (e.g. side-products) are confined to one location. The method provides organometallic compounds in a yield of at least 0.25 (preferably 0.5, especially 1) kg or at least 75 - 99 (preferably 80 - 99)%.

Dwg.0/0

FILE SEGMENT: CPI
 FIELD AVAILABILITY: AB; DCN
 MANUAL CODES: CPI: A05-H01B; A12-W11; A12-W12C; E05-A01; E05-L01;
 E05-M01; E05-M03C; E05-N01; E05-N03A; E05-V01;
 L04-C12; L04-C12A

TECH UPTX: 20050517

TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred Components: The hydrocarbon or heteroatom-containing material is an alcohol, diketone, cyclopentadiene, imine or hydrocarbon (preferably alkoxide, diketone, cyclopentadienide or imide). The base material has a pKa greater than 10 and is selected from **butyl lithium** or **methyl lithium**. The solvent is selected from an optionally saturated hydrocarbon, aromatic hydrocarbon, aromatic heterocycle, alkyl halide, silylated hydrocarbon, ether, polyether, thioether, ester, thioester, lactone, polyamine and/or other aprotic solvents (preferably hexane and/or tetrahydrofuran (THF)).
 Preferred Method: The metal source compound is added to the first reaction mixture at ambient temperature or at a temperature greater than ambient temperature.

TECHNOLOGY FOCUS - INORGANIC CHEMISTRY - Preferred Components: The hydrocarbon or heteroatom-containing material is an amine or halogen (preferably **lithiated amide**). The base material is selected from NaH, CaH or a **lithium amide**. The metal source compound is of formula MX_n (preferably HfCl₄, HfF₄, HfBr₄, HfI₄ or Hf(OTf)₄, especially HfCl₄). The solvent is selected from amide, amine, nitrite and/or silicone oil.
 M = transition metal (preferably hafnium, titanium, zirconium, tantalum or molybdenum);
 X = halide;
 n = 3, 4 or 5.

ABEX UPTX: 20050517

EXAMPLE - To a hexane solution of n-BuLi (**n-butyl lithium**) (3.6 l) was added with stirring, ethylmethylaniline (205 g)

slowly at a rate such that the reaction mixture temperature was kept under 10degreesC. After the addition was complete for 2 hours, the reaction mixture was warmed slowly to 20degreesC and stirring was continued overnight for 16 hours. Anhydrous inhibitor-free tetrahydrofuran (THF) (0.2 l) was added to the white suspension. HfCl₄ (250.1 g) was added slowly (for two hours), and the observed exothermic response registered a maximum temperature of 45degreesC. After the addition, the mixture was allowed to stir for 4 days. After basic work up, tetrakis(ethylmethylamino)hafnium (262 g, 82%) was obtained as a clear, slightly pale-yellow liquid.

L146 ANSWER 83 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
 ACCESSION NUMBER: 2004-682725 [67] WPIX
 DOC. NO. CPI: C2004-243215
 TITLE: Manufacture of perfluoro alkyl imide used as organic ion conductor, involves reacting specific acid anhydride with primary amine, and tertiary amine, heterocyclic amine or aromatic amine in optional presence of solvent.
 DERWENT CLASS: E19
 PATENT ASSIGNEE(S): (KAND) KANTO DENKA KOGYO KK
 COUNTRY COUNT: 1
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
JP 2004269491	A	20040930	(200467)*		13	C07C231-02	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 2004269491	A	JP 2003-324431	20030917

PRIORITY APPLN. INFO: JP 2003-44686 20030221
 INT. PATENT CLASSIF.:

MAIN: C07C231-02
 SECONDARY: C07C231-08; C07C231-12; C07C233-05; C07C235-88;
 C07C303-36; C07C303-38; C07C303-40; C07C311-09;
 C07C311-51; C07F001-02

BASIC ABSTRACT:

JP2004269491 A UPAB: 20041019

NOVELTY - A specific acid anhydride is reacted with primary amine, and tertiary amine, heterocyclic amine or aromatic amine in optional presence of solvent, and perfluoro alkyl imide is obtained.

DETAILED DESCRIPTION - Acid anhydride chosen from formulae: (Rf1Y1)2O and (Rf2Y2)2O is reacted with primary amine of formula: ArCH2NH2, and tertiary amine of formula: R1R2R3N, heterocyclic amine or aromatic amine in optional presence of solvent, and perfluoro alkyl imide of formula: ArCH2N(Y1Rf1)(Y2Rf2) is obtained.

Rf1, Rf2 = 1-6C linear or branched perfluoro alkyl;

Y1, Y2 = CO or SO2;

Ar = (un)substituted aromatic ring; and

R1-R3 = 1-5C alkyl.

INDEPENDENT CLAIMS are included for the following: (i) manufacture of perfluoro alkyl amide of formula: ArCH2NH(Y1Rf1), which involves reacting acid anhydride of formula: (Rf1Y1)2O with primary amine, and tertiary amine, heterocyclic amine or aromatic amine in optional presence of solvent; (ii) manufacture of perfluoro alkyl imide of formula: Rf1Y1-NH-Y2Rf2, which involves oxidizing, reducing or hydrolyzing

perfluoro alkyl imide of formula: $\text{ArCH}_2\text{N}(\text{Y}_1\text{Rf}_1)(\text{Y}_2\text{Rf}_2)$; and (iii) manufacture of perfluoro alkyl imide salt of formula: $\text{M}(\text{Rf}_1\text{Y}_1\text{-N-Y}_2\text{Rf}_2)$, which involves carrying out cation exchange of perfluoro alkyl imide of formula: $\text{Rf}_1\text{Y}_1\text{-NH-Y}_2\text{Rf}_2$.

$\text{Rf}_1, \text{Rf}_2, \text{Y}_1, \text{Y}_2$ = same as defined above.

USE - For manufacturing perfluoro alkyl imide compound used as organic ion conductor, Lewis acid catalyst, and as synthetic intermediate.

ADVANTAGE - The perfluoro alkyl imide compound is easily and economically obtained at high yield and selectivity.

Dwg.0/0

FILE SEGMENT: CPI
FIELD AVAILABILITY: AB; DCN
MANUAL CODES: CPI: E05-A; E10-A08C; E10-A24A; E10-D03D; N02-F02
TECH UPTX: 20041019

TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred Process: Alternately, the perfluoro alkyl imide is obtained by reacting perfluoro alkyl amide with acid anhydride of formula: $(\text{Rf}_2\text{Y}_2)\text{O}$, and tertiary amine, heterocyclic amine or aromatic amine in optional presence of solvent.

Preferred Components: Palladium supporting activated carbon or palladium supporting alumina is used during reduction of perfluoro alkyl imide.

Lithium hydroxide, lithium oxide, lithium

carbonate, lithium chloride and/or lithium hydride is

used during cation exchange of perfluoro alkyl imide.

ABEX UPTX: 20041019

EXAMPLE - Benzylamine (in g) (2.1), triethylamine (2), and methylene chloride (10) was added to trifluoro methanesulfonic acid anhydride (5.6), and stirred for 1 hour. The reaction solution was washed with water (100 mL), and organic layer separated by filtration was dried with magnesium sulfate, and solvent was distilled under reduced pressure. N-benzyl trifluoromethane sulfonamide of formula: $\text{PhCH}_2\text{NHSO}_2\text{CF}_3$ was obtained at yield of 95%.

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ACCESSION NUMBER: 2003-853488 [79] WPIX

DOC. NO. CPI: C2003-240443

TITLE: Production of ethyldimethylamine and triethylamine for use in e.g. surfactants or antioxidants, comprising reacting mixture of diethylamine and dimethylamine with ethylene in presence of sodium diethylamide or dimethylamide.

DERWENT CLASS: B05 D22 D23 E16 F06 M14

INVENTOR(S): BENISCH, C; BOHLING, R; FUNKE, F; GAUS, G; MULLER, G; STEINBRENNER, U; BOEHLING, R; MUELLER, G

PATENT ASSIGNEE(S): (BADI) BASF AG; (BENI-I) BENISCH C; (BOHL-I) BOHLING R; (FUNK-I) FUNKE F; (GAUS-I) GAUS G; (MULL-I) MULLER G; (STEI-I) STEINBRENNER U

COUNTRY COUNT: 103

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
WO 2003074468	A1	20030912	(200379)*	GE	33	C07C209-60	
RW: AT BE BG CH CY CZ DE DK EA EE ES FI FR GB GH GM GR HU IE IT KE LS							
LU MC MW MZ NL OA PT RO SD SE SI SK SL SZ TR TZ UG ZM ZW							
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK							
DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR							
KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT							
RO RU SC SD SE SG SK SL TJ TM TN TR TT TZ UA UG US UZ VC VN YU ZA							
ZM ZW							
DE 10209528	A1	20030918	(200382)			C07C209-60	

AU 2003218681 A1 20030916 (200430) C07C209-60
 EP 1483230 A1 20041208 (200480) GE C07C209-60
 R: AL AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IT LI LT LU LV
 MC MK NL PT RO SE SI SK TR
 KR 2004095260 A 20041112 (200519) C07C209-60
 BR 2003008205 A 20050426 (200530) C07C209-60
 US 2005154235 A1 20050714 (200547) C07C029-08
 JP 2005526743 W 20050908 (200559) 25 C07C209-60
 MX 2004008531 A1 20050101 (200564) C07C209-60
 CN 1649825 A 20050803 (200578) C07C209-60
 ZA 2004007045 A 20051130 (200628) 39 C07C000-00

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2003074468	A1	WO 2003-EP2167	20030303
DE 10209528	A1	DE 2002-10209528	20020304
AU 2003218681	A1	AU 2003-218681	20030303
EP 1483230	A1	EP 2003-711916	20030303
		WO 2003-EP2167	20030303
KR 2004095260	A	KR 2004-713784	20040903
BR 2003008205	A	BR 2003-8205	20030303
		WO 2003-EP2167	20030303
US 2005154235	A1	WO 2003-EP2167	20030303
		US 2004-506514	20040903
JP 2005526743	W	JP 2003-572940	20030303
		WO 2003-EP2167	20030303
MX 2004008531	A1	WO 2003-EP2167	20030303
		MX 2004-8531	20040903
CN 1649825	A	CN 2003-809954	20030303
ZA 2004007045	A	ZA 2004-7045	20040903

FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 2003218681	A1 Based on	WO 2003074468
EP 1483230	A1 Based on	WO 2003074468
BR 2003008205	A Based on	WO 2003074468
JP 2005526743	W Based on	WO 2003074468
MX 2004008531	A1 Based on	WO 2003074468

PRIORITY APPLN. INFO: DE 2002-10209528 20020304

INT. PATENT CLASSIF.:

MAIN: C07C000-00; C07C029-08; C07C209-60
 SECONDARY: C07C209-62; C07C211-04; C07C211-05; C07C211-08;
 C07F001-02; C07F001-04; C07F001-08

BASIC ABSTRACT:

WO2003074468 A UPAB: 20031208

NOVELTY - Ethyldimethylamine and triethylamine are prepared by reacting a mixture of diethylamine and dimethylamine with ethylene in the presence of an alkali metal dimethylamide, diethylamide or hydride catalyst.

DETAILED DESCRIPTION - Ethyldimethylamine (I) and triethylamine (II) are prepared by:

(i) reacting a mixture of diethylamine (III) and dimethylamine (IV) with ethylene in the presence of an alkali metal dimethylamide, diethylamide or hydride catalyst;

(ii) separating off the catalyst;

(iii) separating the resulting mixture by distillation into (I) and

(II) and possibly (III) and (IV); and
(iv) optionally recycling the catalyst and starting amines, to the reaction.

USE - Ethyldimethylamine obtained by this method is used in e.g. the foundry industry (cold-box process), and triethylamine is used for e.g. the production of surfactants, auxiliary materials for textiles and flotation processes, bactericides, corrosion and foam inhibitors, pharmaceutical additives and antioxidants for fats and oils.

ADVANTAGE - The method enables the production of ethyldimethylamine and triethylamine in a single stage, rather than separately, and the two products are easily separated from one another by distillation and the required amounts of each are easily controlled.

Dwg.0/0

FILE SEGMENT: CPI
FIELD AVAILABILITY: AB; DCN
MANUAL CODES: CPI: B10-B04B; B12-M09; B14-A01; B14-S08; D09-A01C;
D10-A03; E10-B04C2; E11-F; F03-C02B; M14-F01; M14-K;
N05-A; N05-D; N07-D

TECH UPTX: 20031208

TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred Method: Reaction is carried out with excess (III), preferably with a ratio of (III)/(II) = (8-15):1, especially 10:1, and also with excess ethylene. The reactor feed stream contains 0-1 (preferably less than 0.1) wt.% ammonia, 0-5 (preferably less than 1) wt.% monoethylamine plus monomethylamine, 20-80 (preferably 40-70) wt.% (III) plus (IV), 0-50 (preferably less than 40) wt.% (II), 5-50 (preferably 10-30) wt.% ethylene, 0.01-20 (preferably 0.1-2) wt.% catalyst and 0-20 wt.% solvent for the catalyst.

Production of the metal amide and hydroamination are carried out in a single stage, and a co-catalyst may also be present. Part of the amine mixture obtained after removing the catalyst is separated off, part of the triethylamine (II) is isomerized by transalkylation with ammonia and the diethylamine obtained is separated and recycled as starting material. Preferred Catalysts: The catalysts are compounds of lithium, sodium or potassium, preferably sodium diethylamide and/or dimethylamide, and are prepared before use from diethylamine or dimethylamine by known methods.

Preferred Co-catalysts: The co-catalysts are cyclic or open-chain imines or tautomeric enamines.

ABEX UPTX: 20031208

EXAMPLE - An autoclave containing sodium diethylamide (50 mmols) was charged with a mixture of diethylamine (5 mols) and dimethylamine (2 mols), heated to 70 degrees C with stirring and pressurized to 40 bar with ethylene. After 360 minutes under these conditions (i.e. with addition of ethylene to maintain the pressure), the reaction mixture (after deactivation of the catalyst with ethanol) contained 66.68% triethylamine and 17.98% N-ethyldimethylamine (by GC peak areas); the amount of ethylene added was 245.5 g and uptake of ethylene was 17.5 g/min at this point. Corresponding values after 30 minutes were 14.35%, 22.89%, 140.5 g and 83.5 g/min.

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ACCESSION NUMBER: 2003-450571 [43] WPIX

DOC. NO. CPI: C2003-119895

TITLE: Production of alkali metal dialkylamide used as catalyst e.g. in trialkylamine production, comprises adding dialkylamine and butadiene in controlled amounts to a suspension of alkali metal in a solvent.

DERWENT CLASS: E12 E16

INVENTOR(S): BOHLING, R; FUNKE, F; HARDER, W; STEINBRENNER, U;
BOEHLING, R; B6HLING, R

PATENT ASSIGNEE(S): (BADI) BASF AG; (BOHL-I) BOHLING R; (FUNK-I) FUNKE F;
 (HARD-I) HARDER W; (STEI-I) STEINBRENNER U
 COUNTRY COUNT: 103
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
DE 10155474	A1	20030522	(200343)*		10	C07F001-00	
WO 2003042154	A2	20030522	(200344)	GE		C07C209-00	
RW: AT BE BG CH CY CZ DE DK EA EE ES FI FR GB GH GM GR IE IT KE LS LU							
MC MW MZ NL OA PT SD SE SK SL SZ TR TZ UG ZM ZW							
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK							
DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR							
KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT							
RO RU SC SD SE SG SI SK SL TJ TM TN TR TT TZ UA UG US UZ VC VN YU							
ZA ZM ZW							
EP 1451141	A2	20040901	(200457)	GE		C07C209-00	
R: AL AT BE BG CH CY CZ DE DK EE ES FI FR GB GR IE IT LI LT LU LV MC							
MK NL PT RO SE SI SK TR							
AU 2002363584	A1	20030526	(200464)			C07C209-00	
US 2005038253	A1	20050217	(200514)			C07F001-04	
JP 2005509020	W	20050407	(200524)		29	C07F001-04	
CN 1639107	A	20050713	(200576)			C07C209-00	
KR 2005044431	A	20050512	(200637)			C07C209-00	
IN 2004001022	P4	20060203	(200639)	EN		C07C209-00	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
DE 10155474	A1	DE 2001-10155474	20011112
WO 2003042154	A2	WO 2002-EP12528	20021108
EP 1451141	A2	EP 2002-798307	20021108
		WO 2002-EP12528	20021108
AU 2002363584	A1	AU 2002-363584	20021108
US 2005038253	A1	WO 2002-EP12528	20021108
		US 2004-495356	20041008
JP 2005509020	W	WO 2002-EP12528	20021108
		JP 2003-543991	20021108
CN 1639107	A	CN 2002-824833	20021108
KR 2005044431	A	WO 2002-EP12528	20021108
		KR 2004-707215	20040512
IN 2004001022	P4	WO 2002-EP12528	20021108
		IN 2004-CN1022	20040512

FILING DETAILS:

PATENT NO	KIND	PATENT NO
EP 1451141	A2 Based on	WO 2003042154
AU 2002363584	A1 Based on	WO 2003042154
JP 2005509020	W Based on	WO 2003042154
KR 2005044431	A Based on	WO 2003042154

PRIORITY APPLN. INFO: DE 2001-10155474 20011112

INT. PATENT CLASSIF.:

MAIN: C07C209-00; C07F001-00; C07F001-04
 SECONDARY: B01J031-02; B01J031-26; C07C209-60; C07C211-03;
 C07C211-35; C07C211-65; C07F001-02; C07F001-06

BASIC ABSTRACT:

DE 10155474 A UPAB: 20030707

NOVELTY - Production of alkali metal dialkylamides (I) comprises reacting a dialkylamine (II) with a metal in the presence of an electron donor, e.g. butadiene, by adding the dialkyl amine, present at 45 weight%, preferably 15 weight%, and the donor, present at 5 weight%, preferably 1.5 weight%,

to suspension of metal in solvent.

DETAILED DESCRIPTION - Production of alkali metal dialkylamides (I) comprises reacting a dialkylamine (II) with an alkali metal in the presence of an electron donor, e.g. 1,3-butadiene (preferred), isoprene, naphthalene and/or styrene, by ad8211

adding the dialkyl amine, present at 45 weight%, preferably 15 weight%, and the donor, present at 5 weight%, preferably 1.5 weight%, to suspension of metal in solvent.

INDEPENDENT CLAIMS are included for:

(1) a mixture containing (I), optionally solvent and secondary amine(s) from this method, in which the mole ratio of total hydroamination product to (I) is less than 1.5, preferably less than 1, most preferably less than 0.3; and

(2) a method for the production of trialkylamines from corresponding dialkylamines and olefins using (I) as catalyst.

USE - Alkali metal dialkylamides obtained by this method are used as catalysts e.g. for the production of trialkylamines from olefins and dialkylamines, especially triethylamine from ethylene and diethylamine.

ADVANTAGE - Enables the production of alkali metal dialkylamide catalysts from metal and dialkylamine in presence of 1,3-butadiene as electron donor, with the formation of only small amounts of the addition product butenyl-dialkylamine.

Dwg.0/0

FILE SEGMENT: CPI

FIELD AVAILABILITY: AB; DCN

MANUAL CODES: CPI: E05-A; E10-B04C2; N05-E01; N06-E01; N07-D08A

TECH UPTX: 20030707

TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred Solvents: The solvent is preferably saturated hydrocarbon, preferably low-boiling paraffins or their mixtures, or high-boiling paraffins (optionally branched and containing saturated cycloparaffins), mono-olefins and/or trialkylamines (as suspending media).

Preferred Amines: The amine is preferably alkylamines with linear or branched, cyclic or acyclic 1-50C alkyl groups (optionally with inert substituents), preferably methyl to pentyl, decyl, dodecyl, hexadecyl, cyclohexyl or cyclopentyl groups, especially amines with hydrogen in the beta-position to the nitrogen, more especially amines with ethyl or n-butyl groups, preferably dialkylamines.

Preferred Olefins: The olefin is preferably 2-20C olefins, preferably ethylene, propylene, 1-butene, 2-butene or cyclohexene, especially ethylene (for reaction to produce trialkylamines).

Preferred Method: The mole ratio of (electron donor):(metal) is 0.5-1.2, preferably 0.5-1.0, especially 0.5-0.7.

TECHNOLOGY FOCUS - INORGANIC CHEMISTRY - Preferred Metals: The metal is preferably sodium, potassium or lithium, especially Na or K, preferably Na, with a particle size distribution such that 50 wt.% of the particles are smaller than 1000 microm (preferably below 300 microm, especially below 100 microm).

ABEX UPTX: 20030707

EXAMPLE - A dispersion of 0.55 mol sodium metal in 220 g n-heptane and 7.001 g n-undecane was treated over 180 minutes at 30 degreesC with a mixture of 0.35 mol 1,3-butadiene and 1.05 mols diethylamine (DEA), so that the butadiene concentration was always below 0.24 wt.% and the DEA

concentration was always below 15 wt.% (mostly below 10 wt.%). GC analysis of the product showed that the amount of addition product (butenyldiethylamine (BueDEA)) was less than 0.0001 g after 11, 41, 60, 90 or 120 minutes. The amount increased to 0.13 g after 150 minutes, to 4.7 g after 180 minutes and to an unacceptable level (13 g) if the addition was continued to 230 minutes. The yield of sodium diethylamide (NaN_{Et}2) was 85 %, with complete conversion of sodium and the mol ratio of (BueDEA):(NaN_{Et}2) was ca. 0.2 after 180 minutes. If the reaction was carried out by adding DEA and butadiene to a dispersion of sodium in DEA and n-undecane, with DEA concentrations decreasing from 96 % to 79 % after 205 hours, the yield of NaN_{Et}2 was only 7 % and the (BueDEA):(NaN_{Et}2) ratio was ca. 15.

L146 ANSWER 86 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
 ACCESSION NUMBER: 2003-156908 [15] WPIX
 DOC. NO. CPI: C2003-040799
 TITLE: Preparation of rac-bicalutamide useful for selectively reducing testosterone level, comprising addition of ethyl-(2-(4-fluorophenyl sulfone))-2-hydroxy propionic acid to 5-amino-2-cyano-benzotrifluoride and butyl lithium in organic solvent.
 DERWENT CLASS: B05
 INVENTOR(S): DOLITZKY, B; REANY, O; SHAMMAI, J; SHAMAI, J
 PATENT ASSIGNEE(S): (BIOG) BIOGAL GYOGYSZERGYAR; (DOLI-I) DOLITZKY B; (REAN-I) REANY O; (SHAM-I) SHAMMAI J; (BIOG) BIOGAL GYOGYSZERGYAR RT; (TEVA-N) TEVA PHARM IND LTD; (TEVA-N) TEVA PHARM USA INC
 COUNTRY COUNT: 101
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
WO 2002100339	A2	20021219	(200315)*	EN	11	A61K000-00	
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SL SZ TR TZ UG ZM ZW							
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ OM PH PL PT RO RU SD SE SG SI SK SL TJ TM TN TR TT TZ UA UG US UZ VN YU ZA ZM ZW							
US 2003045741	A1	20030306	(200320)			C07C315-04	
US 2004044249	A1	20040304	(200417)			C07C317-28	
US 2004059147	A1	20040325	(200422)			C07C317-24	
EP 1406855	A2	20040414	(200426)	EN		C07C069-675	
R: AL AT BE CH CY DE DK ES FI FR GB GR IE IT LI LT LU LV MC MK NL PT RO SE SI TR							
US 6737550	B2	20040518	(200433)			C07C315-04	
AU 2002312431	A1	20021223	(200452)			A61K000-00	
US 2004167349	A1	20040826	(200457)			C07C317-00	
US 2004176633	A1	20040909	(200459)			C07C317-24	
US 2004176638	A1	20040909	(200459)			C07F001-02<--	
US 6797843	B2	20040928	(200465)			C07C315-04	
US 6849763	B2	20050201	(200511)			C07C053-122	
US 6861557	B2	20050301	(200516)			C07C231-02	
US 2005090682	A1	20050428	(200530)			C07C317-34	
AU 2002312431	A8	20051020	(200615)			C07C069-675	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
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WO 2002100339	A2	WO 2002-US18329	20020613
US 2003045741	A1 Provisional	US 2001-298009P	20010613
	Provisional	US 2002-371069P	20020409
		US 2002-170721	20020613
US 2004044249	A1 Provisional	US 2001-298009P	20010613
	Provisional	US 2002-371069P	20020409
	CIP of	US 2002-170721	20020613
		US 2003-606403	20030625
US 2004059147	A1 Provisional	US 2001-298009P	20010613
	Provisional	US 2002-371069P	20020409
	Div ex	US 2002-170721	20020613
		US 2003-668982	20030922
EP 1406855	A2	EP 2002-739801	20020613
		WO 2002-US18329	20020613
US 6737550	B2 Provisional	US 2001-298009P	20010613
	Provisional	US 2002-371069P	20020409
		US 2002-170721	20020613
AU 2002312431	A1	AU 2002-312431	20020613
US 2004167349	A1 Provisional	US 2001-298009P	20010613
	Provisional	US 2002-371069P	20020409
	Div ex	US 2002-170721	20020613
		US 2004-791468	20040301
US 2004176633	A1 Provisional	US 2001-298009P	20010613
	Provisional	US 2002-371069P	20020409
	Div ex	US 2002-170721	20020613
		US 2004-796313	20040308
US 2004176638	A1 Provisional	US 2001-298009P	20010613
	Provisional	US 2002-371069P	20020409
	Div ex	US 2002-170721	20020613
		US 2004-796822	20040308
US 6797843	B2 Provisional	US 2001-298009P	20010613
	Provisional	US 2002-371069P	20020409
	Div ex	US 2002-170721	20020613
		US 2003-668982	20030922
US 6849763	B2 Provisional	US 2001-298009P	20010613
	Provisional	US 2002-371069P	20020409
	Div ex	US 2002-170721	20020613
		US 2004-796822	20040308
US 6861557	B2 Provisional	US 2001-298009P	20010613
	Provisional	US 2002-371069P	20020409
	Div ex	US 2002-170721	20020613
		US 2004-796313	20040308
US 2005090682	A1 Provisional	US 2001-298009P	20010613
	Provisional	US 2002-371069P	20020409
	Div ex	US 2002-170721	20020613
	Div ex	US 2004-791468	20040301
	Div ex	US 2004-796313	20040308
	Div ex	US 2004-796822	20040308
		US 2004-994267	20041123
AU 2002312431	A8	AU 2002-312431	20020613

FILING DETAILS:

PATENT NO	KIND	PATENT NO
EP 1406855	A2 Based on	WO 2002100339
AU 2002312431	A1 Based on	WO 2002100339
US 2004167349	A1 Div ex	US 6737550
US 2004176633	A1 Div ex	US 6737550

US 2004176638	A1 Div ex	US 6737550
US 6797843	B2 Div ex	US 6737550
US 6849763	B2 Div ex	US 6737550
US 6861557	B2 Div ex	US 6737550
US 2005090682	A1 Div ex	US 6737550
	Div ex	US 6849763
	Div ex	US 6861557
AU 2002312431	A8 Based on	WO 2002100339

PRIORITY APPLN. INFO: US 2002-371069P 20020409; US
2001-298009P 20010613; US
2002-170721 20020613; US
2003-606403 20030625; US
2003-668982 20030922; US
2004-791468 20040301; US
2004-796313 20040308; US
2004-796822 20040308; US
2004-994267 20041123

INT. PATENT CLASSIF.:

MAIN: A61K000-00; C07C053-122; C07C069-675; C07C231-02;
C07C315-04; C07C317-00; C07C317-24; C07C317-28;
C07C317-34; C07F001-02

SECONDARY: C07C053-134; C07C231-08; C07C255-49; C07C255-50;
C07C317-14

BASIC ABSTRACT:

WO2002100339 A UPAB: 20030303

NOVELTY - Preparation (P1) of rac-bicalutamide (I) (both R- and S-isomers) comprises addition of ethyl-(2-(4-fluorophenyl sulfone))-2-hydroxy propionic acid (i) to a mixture of 5-amino-2-cyano-benzotrifluoride and **butyl lithium** in an organic solvent, and recovering.

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for the following:

(1) a rac-bicalutamide intermediate of formula (X) or (Y), which represent stable **organo lithium** salts of 4-fluorophenyl methyl sulfone and 5-amino-2-cyano-benzotrifluoride, respectively;

(2) preparation (P2) of the intermediates comprising addition of **butyl lithium** to a solution of a substrate (S1 or S2 representing 4-fluorophenyl methyl sulfone and 5-amino-2-cyano-benzotrifluoride for (X) and (Y) preparation, respectively) in the organic solvent.

(3) preparation (P3) of methyl 2,3-epoxy-2-methyl propionate comprising addition of methyl methacrylate to oxone dissolved in a basic solution, followed by addition of an acid;

(4) preparation (P4) of 2-hydroxy-2-methyl-3-(4-fluorophenylthio)propionic acid comprising addition of methyl-1,2-epoxy-2-methyl propionate to a solution of 4-fluorothiophenol in methanol, followed by addition of ethyl acetate and recovering the product;

(5) preparation of ethyl-(2-(4-fluorophenyl sulfone))-2-hydroxy propionate comprising addition of ethyl pyruvate to a mixture of 4-fluorophenyl methyl sulfone and **butyl lithium** in an organic solvent followed by recovering; and

(6) micronized (I) having a mean particle diameter of less than 200 μ m (preferably less than 100 μ m, especially less than 10 μ m).

ACTIVITY - None given in the source material.

MECHANISM OF ACTION - None given in the source material.

USE - Micronized (I) is used for preparation of a composition (claimed) useful for selectively reducing the testosterone level.

ADVANTAGE - The processes are economical, environmentally safe and feasible. The process is simple without involvement of any dangerous oxidizing compounds such as meta-chloroperbenzoic acid. The mean particle size of (I) provides an improved, reproducible and stable dissolution profile. (I) Also has an anti-androgen activity and selectively decreases the testosterone level without influencing the regulation mechanisms of the hypothalamus. (I) (Particularly the (R) isomer) is more active having lesser side effects such as headache and giddiness.

Dwg.0/2

FILE SEGMENT: CPI
FIELD AVAILABILITY: AB; DCN
MANUAL CODES: CPI: B10-A10; B10-A15; B10-C04B; B14-D02A
TECH UPTX: 20030303

TECHNOLOGY FOCUS - **ORGANIC CHEMISTRY** - Preferred Components: The basic solution is potassium hydroxide or sodium hydroxide (preferably 10M potassium hydroxide for (P3) and 2N sodium hydroxide for (P4)). Oxone is potassium hydrogen sulfate (KHSO5) (50%). The acid is hydrochloric, nitric or phosphoric acid (preferably 0.05 - 5 N hydrochloric acid). Preferred Process: In (P1), (i) is added to the mixture at -65 degrees C. (I) Is obtained by evaporating a reaction mixture, preferably separating (i). In (P2), **butyl lithium** reacts with the substrate in the presence of an anion stabilizer (preferably 1,4-diazabicyclo(2.2.2)octane) at -40 to 10 (preferably -2 to 2) degrees C. In (P3), methyl methacrylate is added in methanol and the oxone solution containing the methyl methacrylate is maintained at pH 6. In (P4), the 4-fluorothiophenol solution is prepared by adding the basic solution under N2 flow. The reaction mixture in (P4) is obtained by stirring at room temperature for 90 minutes. The recovery in (P4) is by extraction (preferably chloroform extraction) and further solidification of the product.

ABEX UPTX: 20030303
SPECIFIC COMPOUNDS - Tetrahydrofuran or diethyl ether are specifically claimed as the organic solvent.

ADMINISTRATION - The dosage of (I) is 2 - 200 (preferably 5 - 100) mg/day and is administered orally or intravenously.

EXAMPLE - 4-Fluorophenyl methyl sulfone (4-FPMS) (5 g) and 1,4-diazabicyclo(2.2.2)octane (3.2 g) (DABCO) were dissolved in tetrahydrofuran (THF) and cooled to -2 degrees C in dry-ice acetone bath. A **butyl lithium** solution (2.5 M) in hexane (14.5 ml) was added to the cold THF dropwise at -2 to 2 degrees C. The mixture was then stirred for 1 hour and then ethyl pyruvate solution (3.67 g) in THF (30 ml) was added to the mixture at -65 degrees C. The mixture was stirred for 1 hour at -65 to -30 degrees C. 2N hydrochloric acid (HCl) was then added to the reaction and the mixture was warmed to room temperature. The reaction mixture was evaporated in vacuo, after which the residue was extracted with diethyl ether (3 x 100 ml). The combined ether extracts were dried over sodium bisulfate (NaSO4), filtered and purified by column chromatography using dichloromethane to give rac-ethyl-(2-(4-fluorophenyl sulfone))-2-hydroxy propionate.

L146 ANSWER 87 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
ACCESSION NUMBER: 2002-547841 [58] WPIX
DOC. NO. CPI: C2002-155384
TITLE: New substituted 1,4,7,10-tetraazacyclododecane **lithium** complexes, are crystalline, easily purified intermediates for gadolinium complex useful in magnetic resonance imaging.
DERWENT CLASS: B03

INVENTOR(S): BLASZKIEWICZ, P; HOFFMANN, H; PETROV, O; PLATZEK, J;
MANN, H; HOFFMAN, H
PATENT ASSIGNEE(S): (SCHD) SCHERING AG
COUNTRY COUNT: 99
PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2002048119	A2	20020620	(200258)	GE	10	C07D257-00
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SL SZ TR TZ UG ZM ZW						
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DK DM DZ EC EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ PH PL PT RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG UZ VN YU ZA ZW						
DE 10064467	A1	20020711	(200258)			C07D257-02
US 2002128472	A1	20020912	(200262)			C07D257-02
AU 2002031659	A	20020624	(200267)			C07D257-00
DE 10064467	C2	20021031	(200273)			C07D257-02
NO 2003002523	A	20030604	(200356)			C07D257-00
EP 1343770	A2	20030917	(200362)	GE		C07D257-00
R: AL AT BE CH CY DE DK ES FI FR GB GR IE IT LI LT LU LV MC MK NL PT RO SE SI TR						
CZ 2003001641	A3	20030917	(200364)			C07D257-00
SK 2003000729	A3	20031104	(200377)			C07D257-00
KR 2003077555	A	20031001	(200410)			C07F001-02<--
HU 2003002563	A2	20031229	(200413)			C07D257-02
JP 2004515545	W	20040527	(200435)		25	C07D257-02
CN 1481371	A	20040310	(200437)			C07D257-02
MX 2003005240	A1	20031101	(200468)			C07D257-00
ZA 2003005421	A	20041124	(200481)		19	C07D000-00
US 6894151	B2	20050517	(200533)			C07F005-00
BR 2001016219	A	20060221	(200617)			C07D257-02
NZ 526478	A	20060428	(200632)			C07D257-00
CN 1229357	C	20051130	(200652)			C07D257-02

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2002048119	A2	WO 2001-EP14283	20011205
DE 10064467	A1	DE 2000-10064467	20001215
US 2002128472	A1 Provisional	US 2000-258311P	20001228
		US 2001-13840	20011213
AU 2002031659	A	AU 2002-31659	20011205
DE 10064467	C2	DE 2000-10064467	20001215
NO 2003002523	A	WO 2001-EP14283	20011205
		NO 2003-2523	20030604
EP 1343770	A2	EP 2001-991788	20011205
		WO 2001-EP14283	20011205
CZ 2003001641	A3	WO 2001-EP14283	20011205
		CZ 2003-1641	20011205
SK 2003000729	A3	WO 2001-EP14283	20011205
		SK 2003-729	20011205
KR 2003077555	A	KR 2003-708035	20030616
HU 2003002563	A2	WO 2001-EP14283	20011205
		HU 2003-2563	20011205
JP 2004515545	W	WO 2001-EP14283	20011205
		JP 2002-549650	20011205
CN 1481371	A	CN 2001-820680	20011205

MX 2003005240	A1	WO 2001-EP14283	20011205
		MX 2003-5240	20030612
ZA 2003005421	A	ZA 2003-5421	20030714
US 6894151	B2 Provisional	US 2000-258311P	20001228
		US 2001-13840	20011213
BR 2001016219	A	BR 2001-16219	20011205
		WO 2001-EP14283	20011205
NZ 526478	A	NZ 2001-526478	20011205
		WO 2001-EP14283	20011205
CN 1229357	C	CN 2001-820680	20011205

FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 2002031659	A Based on	WO 2002048119
EP 1343770	A2 Based on	WO 2002048119
CZ 2003001641	A3 Based on	WO 2002048119
SK 2003000729	A3 Based on	WO 2002048119
HU 2003002563	A2 Based on	WO 2002048119
JP 2004515545	W Based on	WO 2002048119
MX 2003005240	A1 Based on	WO 2002048119
BR 2001016219	A Based on	WO 2002048119
NZ 526478	A Based on	WO 2002048119

PRIORITY APPLN. INFO: DE 2000-10064467 20001215

INT. PATENT CLASSIF.:

MAIN: C07D000-00; C07D257-00; C07D257-02; C07F001-02;
C07F005-00

SECONDARY: A61K031-395; A61K049-10

BASIC ABSTRACT:

WO 200248119 A UPAB: 20020924

NOVELTY - N-(2,3-dihydroxypropyl)-tris-carboxymethyl-tetraazacyclododecane
lithium complexes (I) are new.DETAILED DESCRIPTION - Lithium complexes of formula (I) are
new.X = n Li⁺ ions and m H atoms;

n, m = 0-3 (preferably 0.8-2.2);

m + n = 3; and

Y = Cl or Br.

An INDEPENDENT CLAIM is included for the preparation of (I).

USE - The use of (I) is claimed in the preparation of Gadobutrol
(RTM; N-(1-hydroxymethyl-2,3-dihydroxypropyl)-1,4,7-tris-carboxymethyl-
1,4,7,10-tetraazacyclododecane gadolinium complex) of formula (II), which
is useful in diagnostic imaging, especially magnetic resonance imaging
(MRI); referenced in DE4009119.ADVANTAGE - (I) crystallizes from weakly acidic aqueous ethanol and
is readily isolated in high purity, crystalline form. The lithium
chloride or bromide formed during crystallization remains in solution, and
is readily recovered as lithium hydroxide using an anion
exchanger. By contrast, the preparation of the sodium analogs of (I) (see
DE197241867) requires tedious isolation of sodium chloride from strongly
acidic aqueous methanol. (I) forms the complex (II) with gadolinium
complex in water, and (II) can be recovered in salt-free form (without use
of ion exchangers) by crystallization from aqueous ethanol.

Dwg.0/0

FILE SEGMENT: CPI

FIELD AVAILABILITY: AB; GI; DCN

MANUAL CODES: CPI: B05-A01B; B07-D13

TECH UPTX: 20020924

TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preparation (claimed): Compounds (I) are prepared by reacting N-(6-hydroxy-2,2-dimethyl-1,3-dioxepan-5-yl)-1,4,7,10-tetraazacyclododecane (or its complex with lithium chloride or lithium bromide) with chloro- or bromoacetic acid in a polar solvent at 40-150 degrees C and pH 8-14.

ABEX

UPTX: 20020924

EXAMPLE - A solution chloroacetic acid (38.5 g) in water (40 g) was cooled to 10 degrees C, treated with lithium hydroxide monohydrate (17.1 g) followed by a solution of N-(6-hydroxy-2,2-dimethyl-1,3-dioxepan-5-yl)-1,4,7,10-tetraazacyclododecane (41.25 g) in water (45 ml), heated to 65 degrees C, treated with lithium hydroxide monohydrate (14.6 g) in portions over 2 hours, stirred at 65 degrees C for a further 1 hour, acidified to pH 4 with hydrochloric acid, treated with ethanol (500 ml) over 75 minutes at 65-75 degrees C, boiled under reflux for 2 hours and cooled to room temperature. The obtained crystals were filtered off, washed with 2 x 20 ml 80% and 2 x 20 ml 90% ethanol and dried at 50 degrees C to give N-(1-hydroxymethyl-2,3-dihydroxypropyl)-1,4,7-tris-carboxymethyl-1,4,7,10-tetraazacyclododecane lithium complex (51.6 g, 81.5%) (Ia). A solution of (Ia) (51.6 g) in deionized water (51 g) was adjusted to pH 3.5 with concentrated hydrochloric acid, treated with gadolinium oxide (Gd₂O₃) (16.9 g), stirred for 1 hour at 90 degrees C (adjusting the pH to 7 with solid lithium hydroxide monohydrate if necessary), treated with ethanol (960 ml) over 2 hours at 78 degrees C, boiled under reflux for 5 hours and cooled to room temperature. The obtained crystals were filtered off, washed with ethanol (100 ml) and dried at 50 degrees C to give N-(1-hydroxymethyl-2,3-dihydroxypropyl)-1,4,7-tris-carboxymethyl-1,4,7,10-tetraazacyclododecane gadolinium complex (51.02 g, 85.73%), i.e. Gadobutrol (RTM). Recrystallization from aqueous ethanol gave completely salt-free Gadobutrol (RTM).

DEFINITIONS - Preferred Definitions:

One X group = Li and the other two H; and
Y = Cl.

L146 ANSWER 88 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN

ACCESSION NUMBER: 2003-770425 [73] WPIX

DOC. NO. CPI: C2003-211799

TITLE: Fluorine-containing lithio-oxiranes, useful for the preparation of intermediates for drugs and agricultural chemicals .

DERWENT CLASS: B05 C03

PATENT ASSIGNEE(S): (CENG) CENTRAL GLASS CO LTD

COUNTRY COUNT: 1

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
JP 2002275170	A	20020925	(200373)*		11	C07D303-08	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 2002275170	A	JP 2001-72725	20010314

PRIORITY APPLN. INFO: JP 2001-72725 20010314

INT. PATENT CLASSIF.:

MAIN: C07D303-08
SECONDARY: C07C017-263; C07C022-08; C07C029-32; C07C033-40;
C07C033-48; C07D301-26; C07D303-14; C07F001-02;

C07F005-02; C07F007-08
C07M009:00

INDEX:

BASIC ABSTRACT:

JP2002275170 A UPAB: 20031112

NOVELTY - A chemical species active to an **electrophilic** reagent is new.

DETAILED DESCRIPTION - A chemical species active to an **electrophilic** reagent and stable at -98 deg. C is prepared by reacting an alcohol of formula (X)2CHC(OH)(R2)CF3 (I) with an **organic lithium** compound R2-Li in a solvent.

R1 = alkyl, alkenyl, alkynyl, aryl or heterocyclic ring each optionally substituted;

X = Cl, Br or I; and

R2 = alkyl, alkenyl or aryl.

INDEPENDENT CLAIMS also included for the:

(1) production of an olefin of formula R4C(R2)=C(R1)CF3 (VI); and

(2) production of an olefin of formula R5-CH=CH-C(OH)(R1)CF3 (VII).

USE - The chemical species is used for the preparation of intermediates for drugs and agricultural chemicals.

Dwg.0/0

FILE SEGMENT: CPI

FIELD AVAILABILITY: AB; GI; DCN

MANUAL CODES: CPI: B06-H; B07-A03; B07-H; B10-E04B; B10-E04D; B11-C01C; C06-H; C07-A03; C07-H; C10-E04B; C10-E04D; C11-C01C

TECH UPTX: 20031112

TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preparation: (VI) is prepared by reacting a boron compound of formula R4BZ2 with the above formed chemical species. (VII) is prepared by reacting (I) with R5-(CH)2-Li.

Z = alkyl, alkenyl or alkynyl;

R4, R5 = R1

Preferred Species: The chemical species is an oxirane of formula:

R3 = monovalent organic group based on an **electrophilic** agent or Li.

ABEX UPTX: 20031112

EXAMPLE - A solution of R1MgBr (30 mmol) in tetrahydrofuran was added to 3,3-dichloro-1,1,1-trifluoroacetone (23 ml) at 0 degrees C and the mixture stirred at 0 degrees C for 10-30 minutes. The ice bath was removed and the mixture was stirred overnight, saturated ammonium chloride solution was added and the aqueous solution was extracted with diethyl ether. The extract was dried over magnesium sulfate and concentrated in vacuo and purified by a silica gel column chromatography to give the corresponding alcohol. The corresponding oxirane was derived from the alcohol.

L146 ANSWER 89 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN

ACCESSION NUMBER: 2001-267418 [28] WPIX

DOC. NO. CPI: C2001-081137

TITLE: Ionic metal complex having a novel chemical structure is used as a supporting electrolyte for electrochemical devices, **lithium** (ion) batteries, and electrical double-layer capacitors.

DERWENT CLASS: A17 E12 E19 J03 J04 L03

INVENTOR(S): TAKAHASHI, M; TAKASE, H; TSUJIOKA, S

PATENT ASSIGNEE(S): (CENG) CENTRAL GLASS CO LTD

COUNTRY COUNT: 30

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
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EP 1074555	A2	20010207	(200128)*	EN	14	C07F005-06	
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R: AL AT BE CH CY DE DK ES FI FR GB GR IE IT LI LT LU LV MC MK NL PT

RO SE SI

CA 2314739	A1	20010202 (200128)	EN	C07F005-04
JP 2001106694	A	20010417 (200128)	11	C07F019-00
CN 1282726	A	20010207 (200129)		C07C053-00
KR 2001049956	A	20010615 (200171)		C07F019-00
US 6407232	B1	20020618 (200244)		C07D279-00
KR 367254	B	20030110 (200338)		C07F019-00
JP 2005206611	A	20050804 (200551)	10	C07F005-04
CA 2314739	C	20060124 (200612)	EN	C07F009-00

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
EP 1074555	A2	EP 2000-115578	20000719
CA 2314739	A1	CA 2000-2314739	20000731
JP 2001106694	A	JP 2000-69201	20000313
CN 1282726	A	CN 2000-122469	20000802
KR 2001049956	A	KR 2000-44549	20000801
US 6407232	B1	US 2000-625349	20000725
KR 367254	B	KR 2000-44549	20000801
JP 2005206611	A Div ex	JP 2000-69201	20000313
		JP 2005-114074	20050412
CA 2314739	C	CA 2000-2314739	20000731

FILING DETAILS:

PATENT NO	KIND	PATENT NO
KR 367254	B Previous Publ.	KR 2001049956

PRIORITY APPLN. INFO: JP 2000-69201 20000313; JP
1999-219045 19990802

INT. PATENT CLASSIF.:

MAIN: C07C053-00; C07D279-00; C07F005-04; C07F005-06;
C07F009-00; C07F009-6574; C07F019-00

SECONDARY: C07C053-15; C07C055-00; C07C055-32; C07C057-00;
C07C057-52; C07C059-00; C07C059-135; C07D273-00;
C07D279-04; C07D409-00; C07D493-00; C07F001-00;
C07F001-02; C07F001-08; C07F003-00; C07F003-06;
C07F005-00; C07F005-02; C07F007-00; C07F007-04;
C07F007-07; C07F009-6571

ADDITIONAL: C08F004-06; C08F004-76; C08F010-00; H01M010-40

BASIC ABSTRACT:

EP 1074555 A UPAB: 20010522

NOVELTY - An ionic metal complex having a novel chemical structure is used as a supporting electrolyte for electrochemical devices, **lithium** (ion) batteries, and electrical double-layer capacitors.

DETAILED DESCRIPTION - The ionic metal complex is represented by the formula (1).

M = a transition metal such as elements of groups 3-11 or 12-15 of the periodic table;

Aa+ = a metal ion, onium ion or proton, provided that M is not B when

Aa+ is Cs+;

a = 1-3;

b = 1-3;

p = b/a;

m = 1-3;

n = 0-4;

q = 0-1;

X1 and X2 = O,S or NR5R6;
R1 and R2 = each independently H, a halogen, 1-10C alkyl group or 1-10C halogenated alkyl group;
R3 = 1-10C (halogenated) alkylene group, 4-20C (halogenated) aryl group;
R4 = a halogen, 1-10C (halogenated) alkyl group, 4-20C (halogenated) aryl group, or X2R7;
R5 and R6 = H or 1-10C alkyl group;
R7 = 1-10C (halogenated) alkyl group, 4-20C (halogenated) aryl group.
An INDEPENDENT CLAIM is also included for synthesizing the above ionic metal complex by reacting a compound of the formula (2) with a metal complex represented by the formula (3). (2) contains at least two active hydrogens.

X1,R1-4, M, Aa+, q,a, b, p, m,n = as above;
R8 = a halogen, hydroxyl group, H, 1-10C (halogenated) alkyl group, 4-20C (halogenated) aryl group or X3R9;
X3 = O,S or NR5R6.
R5 and R6 = as above;
R9 = 1-10C (halogenated) alkyl group, 4-20C (halogenated) aryl group.
USE - The metal complex is used as a supporting electrolyte for lithium (ion) batteries, electrical double-layer capacitors and other electrochemical devices.

ADVANTAGE - The complexes are heat resistant, hydrolysis resistant, and have low toxicity and are recyclable.

Dwg.0/0

FILE SEGMENT: CPI
FIELD AVAILABILITY: AB; GI; DCN
MANUAL CODES: CPI: A02-A06; A04-G01A; E05-A; E05-B02; E05-B03; E05-C01; E05-D; E05-E01; E05-F; E05-G01; E05-G07; E05-H; E05-J; E05-L; E05-M; E05-N; E05-P; J03-A; J04-X; L03-B03A; L03-E01C

TECH UPTX: 20010522
TECHNOLOGY FOCUS - ORGANIC CHEMISTRY - Preferred Process: Reacting is conducted in a solvent having a dielectric constant of at least 2 at 0-80 degreesC.

ABEX UPTX: 20010522
EXAMPLE - In a glove box having an atmosphere of a dew point of -50 degreesC, 20.2 g of hexafluoro-2-hydroxyisobutyric acid ($\text{HOC}(\text{CF}_3)_2\text{COOH}$) were dissolved in 20 ml of dimethyl carbonate. Next, 6.8 g of lithium tetrakis(methoxy)borate ($\text{LiB}(\text{OCH}_3)_4$) were slowly added to this solution. After this addition, the solution was heated to 60 degreesC and reacted for 3 hours. Dimethyl carbonate was removed the solution at 170 degreesC and 1 Torr, thereby obtaining 20.0 g of a white solid as a product. The product was identified by NMR and elementary analysis as being $\text{LiB}(\text{OC}(\text{CF}_3)_2\text{COO})_2$ having the following formula.

L146 ANSWER 90 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN

ACCESSION NUMBER: 2001-148295 [16] WPIX

DOC. NO. NON-CPI: N2001-108678

DOC. NO. CPI: C2001-044118

TITLE: Preparation of benzene sulfonate lithium complex salts used in electrochemical cells comprises reacting substituted phenol with chlorosulfonic acid, isolating the intermediate and reacting with lithium tetramethanol borate.

DERWENT CLASS: E19 L03 X16

INVENTOR(S): DE MEIJERE, A; LEONOV, A; SCHMIDT, M; DEMEJER, A; RIAONOF, A; SCHMIT, M; DEMEIJERE, A; ANDREI, L; MEIJERE, A D

PATENT ASSIGNEE(S): (MERE) MERCK PATENT GMBH; (DMEI-I) DE MEIJERE A; (LEON-I)

LEONOV A; (SCHM-I) SCHMIDT M; (MEIJ-I) MEIJERE A D
32

COUNTRY COUNT:

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
DE 19932317	A1	20010111	(200116)	*	7	C07F005-02	
EP 1069128	A2	20010117	(200116)	GE		C07F005-04	
R: AL AT BE CH CY DE DK ES FI FR GB GR IE IT LI LT LU LV MC MK NL PT							
RO SE SI							
CA 2313603	A1	20010110	(200117)	EN		C07F005-04	
BR 2000002667	A	20010313	(200118)			C07F001-02<--	
CN 1280130	A	20010117	(200128)			C07F005-04	
JP 2001055396	A	20010227	(200128)		9	C07F019-00	
KR 2001049741	A	20010615	(200171)			C07F005-04	
US 6441216	B1	20020827	(200259)			C07F005-04	
US 2003028023	A1	20030206	(200313)			H01M006-18	
US 6657072	B2	20031202	(200379)			C07F007-02	
US 2004091785	A1	20040513	(200432)			C07F005-02	
EP 1069128	B1	20041110	(200473)	GE		C07F005-04	
R: DE FR GB							
DE 50008571	G	20041216	(200482)			C07F005-04	
RU 2246499	C2	20050220	(200515)			C07F019-00	
US 6864017	B2	20050308	(200518)			H01M006-04	
CN 1177849	C	20041201	(200618)			C07F005-04	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
DE 19932317	A1	DE 1999-1032317	19990710
EP 1069128	A2	EP 2000-113144	20000629
CA 2313603	A1	CA 2000-2313603	20000707
BR 2000002667	A	BR 2000-2667	20000710
CN 1280130	A	CN 2000-120406	20000706
JP 2001055396	A	JP 2000-203763	20000705
KR 2001049741	A	KR 2000-39039	20000708
US 6441216	B1	US 2000-613293	20000710
US 2003028023	A1 Div ex	US 2000-613293	20000710
		US 2002-191479	20020710
US 6657072	B2 Div ex	US 2000-613293	20000710
		US 2002-191479	20020710
US 2004091785	A1 Div ex	US 2000-613293	20000710
	Div ex	US 2002-191479	20020710
		US 2003-697046	20031031
EP 1069128	B1	EP 2000-113144	20000629
DE 50008571	G	DE 2000-00008571	20000629
		EP 2000-113144	20000629
RU 2246499	C2	RU 2000-117945	20000710
US 6864017	B2 Div ex	US 2000-613293	20000710
	Div ex	US 2002-191479	20020710
		US 2003-697046	20031031
CN 1177849	C	CN 2000-120406	20000706

FILING DETAILS:

PATENT NO	KIND	PATENT NO
US 2003028023	A1 Div ex	US 6441216
US 6657072	B2 Div ex	US 6441216

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L146 ANSWER 91 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
 ACCESSION NUMBER: 2001-102279 [11] WPIX
 DOC. NO. CPI: C2001-029801
 TITLE: New aluminosiloxane compound useful as siloxylating agent
 for e.g. the surface of glass products made from metallic
 silicate, thermosetting resins, cellulose, epoxy and
 pigments.
 DERWENT CLASS: A26 E11 G02
 INVENTOR(S): HAN, J R; YANG, J G; HAN, J; YANG, J
 PATENT ASSIGNEE(S): (HANJ-I) HAN J; (YANG-I) YANG J; (HANJ-I) HAN J R;
 (YANG-I) YANG J G
 COUNTRY COUNT: 94
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
WO 2000071553	A1	20001130	(200111)*	EN	38	C07F007-18	
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SL SZ TZ UG ZW							
W: AE AG AL AM AT AU AZ BA BB BG BR BY CA CH CN CR CU CZ DE DK DM DZ EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX NO NZ PL PT RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG US UZ VN YU ZA ZW							
AU 2000046215	A	20001212	(200115)				
KR 2000077357	A	20001226	(200134)			C08G077-00	
EP 1189909	A1	20020327	(200229)	EN		C07F007-18	
R: AL AT BE CH CY DE DK ES FI FR GB GR IE IT LI LT LU LV MC MK NL PT RO SE SI							
KR 333404	B	20020425	(200270)			C08G077-00	
US 6495708	B1	20021217	(200307)			C07F005-06	
JP 2003500411	W	20030107	(200314)		43	C07F019-00	
EP 1189909	B1	20031022	(200373)	EN		C07F007-18	
R: AT BE CH CY DE DK ES FI FR GB GR IE IT LI LU MC NL PT SE							
DE 60006111	E	20031127	(200403)			C07F007-18	
JP 3643535	B2	20050427	(200529)		24	C07F019-00	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2000071553	A1	WO 2000-KR506	20000520
AU 2000046215	A	AU 2000-46215	20000520
KR 2000077357	A	KR 2000-27200	20000520
EP 1189909	A1	EP 2000-927910	20000520
		WO 2000-KR506	20000520
KR 333404	B	KR 2000-27200	20000520
US 6495708	B1	WO 2000-KR506	20000520
		US 2001-762947	20010214
JP 2003500411	W	JP 2000-619809	20000520
		WO 2000-KR506	20000520
EP 1189909	B1	EP 2000-927910	20000520
		WO 2000-KR506	20000520
DE 60006111	E	DE 2000-00006111	20000520
		EP 2000-927910	20000520
		WO 2000-KR506	20000520
JP 3643535	B2	JP 2000-619809	20000520
		WO 2000-KR506	20000520

FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 2000046215	A Based on	WO 2000071553
EP 1189909	A1 Based on	WO 2000071553
KR 333404	B Previous Publ.	KR 2000077357
US 6495708	B1 Based on	WO 2000071553
JP 2003500411	W Based on	WO 2000071553
EP 1189909	B1 Based on	WO 2000071553
DE 60006111	E Based on	EP 1189909
	Based on	WO 2000071553
JP 3643535	B2 Previous Publ.	JP 2003500411
	Based on	WO 2000071553

PRIORITY APPLN. INFO: KR 1999-18491 19990521

INT. PATENT CLASSIF.:

MAIN: C07F007-18; C07F019-00; C08G077-00
 SECONDARY: C07F007-08; C08G077-58; C08G079-10
 ADDITIONAL: C07F001-02; C07F005-06; C07F007-21

BASIC ABSTRACT:

WO 200071553 A UPAB: 20010224

NOVELTY - Aluminosiloxane compounds of formula (I) and (II) are new.

DETAILED DESCRIPTION - Aluminosiloxane compound of formula (I) is new.

R = 1-6C alkyl or phenyl; and

n = 6 - 90.

INDEPENDENT CLAIMS are also included for

(a) An aluminosiloxane compound of formula (II).

M = alkali metal.

(b) Processes for preparing (I) and (II).

(c) A siloxylating agent comprising (I) or (II).

USE - As siloxylating agent for the surface of glass products made from metallic silicate, thermosetting resins, cellulose, epoxy, pigments made from various metallic oxides and other microorganisms.

ADVANTAGE - The aluminosiloxane compounds are prepared from waste silicone compounds and have improved gloss, flexibility, water repellent heat stability and weatherability. This decreases the pollution caused by such compounds.

Dwg.0/7

FILE SEGMENT: CPI

FIELD AVAILABILITY: AB; GI; DCN

MANUAL CODES: CPI: A06-A00E1; A10-E14; A10-E22; A12-B01C; A12-B05; E05-A; E05-B03; E05-E01; E05-E02C; G02-A05

TECH UPTX: 20010224

TECHNOLOGY FOCUS - POLYMERS - Preparation: Compound (II) is prepared as follows:

(A) The siloxane alkali metal salt of formula (III).

R' = H or R; and

m = 3 - 6

is reacted with aluminum compound and secondary or tertiary alcohol to produce a hydrophilic compound of formula (IV)

R'' = R' or M (at least one R'' is different from R');

m' = numbers which make n from 6-90.

(B) compound (IV) is reacted with hydrohalic acid at pH 7-8 to produce an oil-miscible compound of formula (V);

(C) compound (V) is heated to 80-220 degreesC.

Compound (I) is prepared as follows: compound (II) is reacted with (1) compound of formula (VI)

NR'3HX (VI)

X = halogen

in a non polar solvent or (2) compound of formula (VII)

R''' = 1-6C alkyl

is reacted with aluminum compound and secondary or tertiary alcohol. The alcohol is then removed.

Preferred Process: The n value in compound (II) finally produced is adjusted by controlling the amount of aluminum compound used in step (A). The aluminum compound is used in an amount to make the Si/Al mole ratio in compound (II) 12-180 in step (A). Aluminum metal, hydroxide, oxide, alkali metal salt, halide or inorganic acid salt of aluminum is used as the aluminum compound in step (A). In step (B) a basic compound (preferably ammonia gas or ammonia water) is added to the reaction solution containing the compound (IV) to make the solution alkaline. Then hydrohalic acid (preferably hydrochloric acid, hydrobromic acid or hydroiodic acid) is added to control the pH to 7-8. Compound (VI) is used in an equimolar amount to the compound (II). Step (2) is carried out at 60-80 degreesC.

TECHNOLOGY FOCUS - INORGANIC CHEMISTRY - Preferred Reagents: The aluminum compound is aluminum metal, hydroxide, oxide, alkali metal salt, halide or inorganic acid salt of aluminum. The basic compound is ammonia gas or ammonia water. The hydrohalic acid is HCl, HBr or HI.

ABEX

UPTX: 20010224

EXAMPLE - Siloxane alkali metal salt of formula $(\text{CH}_3)_2\text{CH-O-(Si(CH}_3)_2\text{O)}_3\text{-Na}$ (IIIa) (100 ml) was concentrated to 50% siloxane content. To this was added sodium aluminate (6 g), distilled water (3 ml) and isopropyl alcohol (50 ml). The mixture was stirred vigorously for 3 hours, for 1 hour at 40 degreesC and then for one hour at 60 degreesC. To the pale-brown transparent liquid was added the compound (IIIa) (30 ml) to give a hydrophilic aluminosiloxane metal salt. To the salt (IV) was added 28% ammonia water (20 ml) and stirred for 2 hours. Concentrated hydrochloric acid was slowly added dropwise under stirring to get 7.7 pH. The solution was stirred for one hour at 60 degreesC and cooled. n-Hexane (100 ml) was added, the solution stirred for 30 minutes and allowed to stand. The lower layer was extracted with n-hexane, combined with the supernatant and washed with distilled water. The solvent was evaporated to give oil-miscible aluminosiloxane compound. This compound was heated to 150 degreesC to concentrate it. This was then cooled to give aluminosiloxane compound in the gel form. The concentrate was dissolved in n-hexane (300 ml). Ammonium chloride (3 g) was added and the mixture stirred for 4 hours. The supernatant was separated and heated to 150 degreesC to give aluminosiloxane compound (59 g) of average molecular weight 1000. This was heated at 30-40 degreesC for 24 hours and dried. 10 g of the compound was dissolved in xylene (30 ml). YD-011 (epoxy resin) with 800-1000 average molecular weight, prepared from bisphenol A and epichlorohydrin (2 g) was dissolved in the xylene. The solution was heated at 140-150 degreesC for 20 minutes and stirred to cool. G-1034 (hardening agent) (0.25 parts by weight) was added. Surface of flat glass was coated with the product in 0.3 - 0.4 μ thickness. The layer was hardened for 4 days. Adhesion force of the coating layer with the surface of glass was increased. No silicon oil separated from the surface. The surface was more elastic than that coated with epoxy resin which was not siloxylated. Also, the surface gloss was excellent.

L146 ANSWER 92 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN

ACCESSION NUMBER: 1998-286367 [25] WPIX

DOC. NO. CPI: C1998-088579

TITLE: Stereospecific preparation of chiral 1-aryl- and 1-hetero aryl-2-substituted ethyl-2-amine compounds - by reacting chiral 2-amino-2-substituted ethyl alcohol with e.g. (tri halomethyl)sulphonyl halide giving aziridine intermediate, followed by conversion to lithium

salt intermediate.
 DERWENT CLASS: B03 B05
 INVENTOR(S): CASIMIR, J; GRONDARD, L; LEON, P; OBRIEN, M K; POWERS, M R; ROBIN, D; O'BRIEN, M K
 PATENT ASSIGNEE(S): (AVET) AVENTIS PHARM PROD INC; (RHON) RHONE-POULENC RORER PHARM INC; (AVET) AVENTIS PHARM CO; (AVET) AVENTIS PHARM INC
 COUNTRY COUNT: 79
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
WO 9811064	A1	19980319	(199825)*	EN	15	C07C303-38	
RW: AT BE CH DE DK EA ES FI FR GB GH GR IE IT KE LS LU MC MW NL OA PT SD SE SZ UG ZW							
W: AL AM AT AU AZ BA BB BG BR BY CA CN CU CZ DE DK EE ES FI GB GE GH HU IL IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MD MG MK MN MW MX NO NZ PL PT RO RU SD SE SG SI SK SL TJ TM TR TT UA UG US UZ VN YU ZW							
AU 9742562	A	19980402	(199833)			C07C303-38	
NO 9901023	A	19990302	(199924)			C07C303-38	
EP 942900	A1	19990922	(199943)	EN		C07C303-38	
R: AT BE CH DE DK ES FI FR GB GR IE IT LI LU MC NL PT RO SE SI							
SK 9900269	A3	19991008	(199952)			C07C303-38	
BR 9711466	A	19990824	(200001)			C07C303-38	
CN 1230176	A	19990929	(200003)			C07C303-38	
CZ 9900721	A3	20000712	(200040)			C07C303-38	
US 6127550	A	20001003	(200050)			C07D333-20	
MX 9902406	A1	19990801	(200063)			C07C303-38	
HU 2000000219	A2	20001228	(200111)			C07C303-38	
KR 2000036007	A	20000626	(200111)			C07C303-38	
JP 2001501922	W	20010213	(200112)		18	C07C213-00	
AU 732332	B	20010412	(200128)			C07C303-38	
KR 317871	B	20020118	(200254)			C07C303-38	
US 6433172	B1	20020813	(200255)			C07D221-18	
CN 1388119	A	20030101	(200328)			C07D203-24	
IL 128813	A	20050220	(200522)			C07C209-88	
CN 1112354	C	20030625	(200545)			C07C303-40	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 9811064	A1	WO 1997-US15729	19970910
AU 9742562	A	AU 1997-42562	19970910
NO 9901023	A	WO 1997-US15729	19970910
		NO 1999-1023	19990302
EP 942900	A1	EP 1997-940882	19970910
		WO 1997-US15729	19970910
SK 9900269	A3	WO 1997-US15729	19970910
		SK 1999-269	19970910
BR 9711466	A	BR 1997-11466	19970910
		WO 1997-US15729	19970910
CN 1230176	A	CN 1997-197895	19970910
CZ 9900721	A3	WO 1997-US15729	19970910
		CZ 1999-721	19970910
US 6127550	A	Provisional	US 1996-26005P
		Cont of	WO 1997-US15729
			US 1999-266641
MX 9902406	A1	MX 1999-2406	19990311

HU 2000000219	A2	WO 1997-US15729	19970910
		HU 2000-219	19970910
KR 2000036007	A	WO 1997-US15729	19970910
		KR 1999-701970	19990309
JP 2001501922	W	WO 1997-US15729	19970910
		JP 1998-513724	19970910
AU 732332	B	AU 1997-42562	19970910
KR 317871	B	WO 1997-US15729	19970910
		KR 1999-701970	19990309
US 6433172	B1 Provisional	US 1996-26005P	19960912
	Cont of	WO 1997-US15729	19970910
	Div ex	US 1999-266641	19990311
		US 1999-426403	19991025
CN 1388119	A Div ex	CN 1997-197895	19970910
		CN 2001-143342	19970910
IL 128813	A	IL 1997-128813	19970910
CN 1112354	C	CN 1997-197895	19970910

FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 9742562	A Based on	WO 9811064
EP 942900	A1 Based on	WO 9811064
BR 9711466	A Based on	WO 9811064
CZ 9900721	A3 Based on	WO 9811064
HU 2000000219	A2 Based on	WO 9811064
KR 2000036007	A Based on	WO 9811064
JP 2001501922	W Based on	WO 9811064
AU 732332	B Previous Publ.	AU 9742562
	Based on	WO 9811064
KR 317871	B Previous Publ.	KR 2000036007
	Based on	WO 9811064
US 6433172	B1 Div ex	US 6127550
IL 128813	A Based on	WO 9811064

PRIORITY APPLN. INFO: US 1996-26005P 19960912; US
 1999-266641 19990311; US
 1999-426403 19991025

INT. PATENT CLASSIF.:

MAIN: C07C209-88; C07C213-00; C07C303-38; C07C303-40;
 C07D203-24; C07D221-18; C07D333-20

SECONDARY: C07B053-00; C07C211-26; C07C211-27; C07C215-08;
 C07C303-00; C07C307-00; C07C311-03; C07C311-16;
 C07D203-04; C07D333-04; C07D333-28; C07F001-02

INDEX: C07M007:00

BASIC ABSTRACT:

WO 9811064 A UPAB: 19980624

The stereospecific preparation of a ((1-optionally substituted aryl)- or (1-optionally substituted heteroaryl))-2-substituted ethyl-2-amine (I), with chirality at the 2-position, comprises reacting a 2-amino-2-substituted ethyl alcohol, with chirality at the 2-position, with an ((optionally substituted aryl)- or (trihalomethyl) sulphonyl)-halide or anhydride in the presence of a base to form an ((N-arylsulphonyl)- or (N-trihalomethylsulphonyl))-2-substituted aziridine with chirality at the 2-position.

USE - (I) are useful as intermediates in the synthesis of cardiovascular agents, including antihypertensive agents, antiischaemic agents, cardioprotective agents which ameliorate ischaemic injury of myocardial infarct size consequent to myocardial ischaemia, and

antilipolytic agents which reduce plasma lipid levels, serum triglyceride levels and plasma cholesterol levels, and also of agents for treating central nervous system conditions e.g. schizophrenia and epilepsy.

Dwg.0/0

FILE SEGMENT: CPI
FIELD AVAILABILITY: AB; DCN
MANUAL CODES: CPI: B07-H; B10-B04B

L146 ANSWER 93 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
ACCESSION NUMBER: 1998-145231 [13] WPIX
DOC. NO. CPI: C1998-047438
TITLE: Production of baccatin III, used in production of antitumour agents - by reacting 10-de-acetyl-baccatin III with a lithium base and then with an acylating agent.
DERWENT CLASS: B02
INVENTOR(S): SISTI, N J
PATENT ASSIGNEE(S): (NAPR-N) NAPRO BIO THERAPEUTICS INC
COUNTRY COUNT: 79
PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
WO 9802427	A1	19980122	(199813)*	EN	14	C07D305-14	
RW: AT BE CH DE DK EA ES FI FR GB GH GR IE IT KE LS LU MC MW NL OA PT SD SE SZ UG ZW							
W: AL AM AT AU AZ BA BB BG BR BY CA CH CN CU CZ DE DK EE ES FI GB GE GH HU IL IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MD MG MK MN MW MX NO NZ PL PT RO RU SD SE SG SI SK SL TJ TM TR TT UA UG US UZ VN YU ZW							
AU 9738002	A	19980209	(199823)			C07D305-14	
US 5750736	A	19980512	(199826)			C07D305-14	
NZ 333889	A	19990329	(199918)			C07D305-14	
NO 9806066	A	19990305	(199919)			C07D000-00	
EP 918764	A1	19990602	(199926)	EN		C07D305-14	
R: AL AT BE CH DE DK ES FI FR GB GR IE IT LI LT LU LV MC NL PT RO SE SI							
CN 1225089	A	19990804	(199949)			C07D305-14	
BR 9710234	A	20000111	(200020)			C07D305-14	
JP 2000514458	W	20001031	(200059)		13	C07D305-14	
KR 2000023649	A	20000425	(200107)			C07D305-14	
AU 731651	B	20010405	(200125)			C07D305-14	
MX 9900448	A1	20001101	(200163)			C07D305-14	
IL 127850	A	20011125	(200215)			C07D305-14	
EP 918764	B1	20040512	(200431)	EN		C07D305-14	
R: AL AT BE CH DE DK ES FI FR GB GR IE IT LI LT LU LV MC NL PT RO SE SI							
DE 69729100	E	20040617	(200440)			C07D305-14	
CN 1096453	C	20021218	(200528)			C07D305-14	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 9802427	A1	WO 1997-US12307	19970709
AU 9738002	A	AU 1997-38002	19970709
US 5750736	A	US 1996-678759	19960711
NZ 333889	A	NZ 1997-333889	19970709
		WO 1997-US12307	19970709
NO 9806066	A	WO 1997-US12307	19970709

EP 918764	A1	NO 1998-6066	19981222
		EP 1997-934954	19970709
		WO 1997-US12307	19970709
CN 1225089	A	CN 1997-196319	19970709
BR 9710234	A	BR 1997-10234	19970709
		WO 1997-US12307	19970709
JP 2000514458	W	WO 1997-US12307	19970709
		JP 1998-506245	19970709
KR 2000023649	A	KR 1999-700102	19990108
AU 731651	B	AU 1997-38002	19970709
MX 9900448	A1	MX 1999-448	19990108
IL 127850	A	IL 1997-127850	19970709
EP 918764	B1	EP 1997-934954	19970709
		WO 1997-US12307	19970709
DE 69729100	E	DE 1997-629100	19970709
		EP 1997-934954	19970709
		WO 1997-US12307	19970709
CN 1096453	C	CN 1997-196319	19970709

FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 9738002	A Based on	WO 9802427
NZ 333889	A Based on	WO 9802427
EP 918764	A1 Based on	WO 9802427
BR 9710234	A Based on	WO 9802427
JP 2000514458	W Based on	WO 9802427
AU 731651	B Previous Publ. Based on	AU 9738002 WO 9802427
IL 127850	A Based on	WO 9802427
EP 918764	B1 Based on	WO 9802427
DE 69729100	E Based on Based on	EP 918764 WO 9802427

PRIORITY APPLN. INFO: US 1996-678759 19960711

INT. PATENT CLASSIF.:

MAIN: C07D000-00; C07D305-14

SECONDARY: C07F001-02

BASIC ABSTRACT:

WO 9802427 A UPAB: 19980330

Preferential acylation of 10-deacetyl-baccatin III at a C-10 position rather than a C-7 hydroxy position, comprises: (a) dissolving a selected quantity of 10-deacetyl-baccatin III of formula (Ia) in an ether solvent to form a first solution at a first temperature; (b) mixing at least one equivalent of a lithium base into the first solution to form a second solution; (c) adding at least an equivalent of an acylating agent to the second solution at a second temperature to form a third solution; and (d) quenching the third solution with a quenching compound that is effective to eliminate excess lithium base and the acylating agent, to produce a fourth solution containing baccatin III of formula (Ib). Also claimed is an intermediate of formula (Ic) for production of baccatin III. Q = OH in (Ia); OAc in (Ib); and Li+O- in (Ic).

USE - Baccatin III is used in production of antitumour agents.

ADVANTAGE - The process avoids the necessity of protecting the C-7 hydroxy position of 10-deacetyl-baccatin III and deprotecting following the acylation at the C-10 position. The process is relatively inexpensive.

Dwg.0/0

FILE SEGMENT: CPI

FIELD AVAILABILITY: AB; GI; DCN

MANUAL CODES: CPI: B06-A03

L146 ANSWER 94 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN

ACCESSION NUMBER: 1999-025727 [03] WPIX

DOC. NO. CPI: C1999-008092

TITLE: Preparation of mono- and di substituted
N-hydroxyalkyl-tetra aza-cyclododecane derivatives used
in preparation of NMR diagnostic agents - comprises
reaction of 1,4,7,10-tetra aza-cyclododecane with epoxide
in the presence of a lithium salt..

DERWENT CLASS: B03

INVENTOR(S): BLASZKIEWICZ, P; PETROV, O

PATENT ASSIGNEE(S): (SCHD) SCHERING AG

COUNTRY COUNT: 83

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
DE 19724186	A1	19981203	(199903)*		5	C07D257-02	
WO 9855467	A1	19981210	(199904)	GE		C07D257-02	
RW:	AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW NL						
OA	PT SD SE SZ UG ZW						
W:	AL AM AT AU AZ BA BB BG BR BY CA CH CN CU CZ DK EE ES FI GB GE GH						
HU IL IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MD MG MK MN MW MX							
NO NZ PL PT RO RU SD SE SG SI SK SL TJ TM TR TT UA UG UZ VN YU ZW							
ZA 9804734	A	19990331	(199918)		19	C07D000-00	
AU 9884327	A	19981221	(199919)			C07D257-02	
US 5994536	A	19991130	(200003)			C07D487-22	
NO 9905870	A	20000201	(200017)			C07D000-00	
EP 986548	A1	20000322	(200019)	GE		C07D257-02	
R:	AL AT BE CH DE DK ES FI FR GB GR IE IT LI LT LU LV MC NL PT RO SE						
SI							
MX 9910356	A1	20000401	(200124)			C07D257-02	
JP 2002508755	W	20020319	(200222)		21	C07D257-02	
TW 450965	A	20010821	(200239)			C07D257-02	
DE 19724186	C2	20020718	(200249)			C07D257-02	
NO 313459	B1	20021007	(200273)			C07D257-02	
EP 986548	B1	20030730	(200356)	GE		C07D257-02	
R:	AL AT BE CH DE DK ES FI FR GB GR IE IT LI LT LU LV MC NL PT RO SE						
SI							
DE 59809163	G	20030904	(200360)			C07D257-02	
MX 208745	B	20020704	(200366)			C07D257-02	
ES 2205523	T3	20040501	(200431)			C07D257-02	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
DE 19724186	A1	DE 1997-1024186	19970602
WO 9855467	A1	WO 1998-DE1523	19980528
ZA 9804734	A	ZA 1998-4734	19980602
AU 9884327	A	AU 1998-84327	19980528
US 5994536	A	US 1998-88700	19980602
NO 9905870	A	WO 1998-DE1523	19980528
		NO 1999-5870	19991201
EP 986548	A1	EP 1998-934857	19980528
		WO 1998-DE1523	19980528
MX 9910356	A1	MX 1999-10356	19991111
JP 2002508755	W	WO 1998-DE1523	19980528
		JP 1999-501299	19980528

TW 450965	A	TW 1998-108521	19980601
DE 19724186	C2	DE 1997-1024186	19970602
NO 313459	B1	WO 1998-DE1523	19980528
		NO 1999-5870	19991201
EP 986548	B1	EP 1998-934857	19980528
		WO 1998-DE1523	19980528
DE 59809163	G	DE 1998-509163	19980528
		EP 1998-934857	19980528
		WO 1998-DE1523	19980528
MX 208745	B	WO 1998-DE1523	19980528
		MX 1999-10356	19991111
ES 2205523	T3	EP 1998-934857	19980528

FILING DETAILS:

PATENT NO	KIND	PATENT NO
AU 9884327	A Based on	WO 9855467
EP 986548	A1 Based on	WO 9855467
JP 2002508755	W Based on	WO 9855467
NO 313459	B1 Previous Publ.	NO 9905870
EP 986548	B1 Based on	WO 9855467
DE 59809163	G Based on	EP 986548
	Based on	WO 9855467
ES 2205523	T3 Based on	EP 986548

PRIORITY APPLN. INFO: DE 1997-19724186 19970602

INT. PATENT CLASSIF.:

MAIN: C07D000-00; C07D257-02; C07D487-22
 SECONDARY: C07D405-04; C07F001-02; C07F009-6524;
 C07F009-655

BASIC ABSTRACT:

DE 19724186 A UPAB: 19990122

The following are claimed: (i) preparation of 1,4,7,10-tetraazacyclododecane compounds of formula (Ia) comprising reaction of 1,4,7,10-tetraazacyclododecane (optionally in the form of a salt) with an epoxide of formula (II) (in which hydroxy groups are optionally protected), in the presence of 0.8-1.1 (preferably 0.9-1.0) moles of a lithium salt at 40-150 deg. C; (ii) preparation of 1,4,7,10-tetraazacyclododecane compounds of formula (Ib), comprising reaction of 1,4,7,10-tetraazacyclododecane (optionally in the form of a salt) with (II) (in which hydroxy groups are optionally protected), in the presence of more than 1.11 (preferably 1.11-3.0) moles of a lithium salt at 40-150 deg. C; (iii) lithium complexes of (Ia) and (Ib); (iv) N-(6-hydroxy-2,2-dimethyl-1,3-dioxepan-5-yl)-1,4,7,10-tetraazacyclododecane (Ia') and N-(6-hydroxycyclohexyl)-1,4,7,10-tetraazacyclododecane (Ia''). R1 = -CH(R3)CH(R2)OH; R2, R3 = H; or R2+R3 = 4-7 membered ring which optionally contains 1-3 O atoms and is optionally substituted by 1-12C alkyl (itself optionally substituted by 1-3 1-6C alkyl or by 1-3 optionally protected OH groups).

USE- Mono- and disubstituted N- beta -hydroxyalkyl-1,4,7,10-tetraazacyclododecane derivatives are useful as intermediates in preparation of NMR diagnostic agents (see DE-A1 3625417 and EP448191).

ADVANTAGE- The process allows direct mono- and dialkylation of the tetraazacyclododecane ring and does not require difficult protection steps required in prior art processes. The use of varying amounts of the lithium salt allows the selectivity of the alkylation to be controlled.

Dwg.0/0

FILE SEGMENT: CPI

FIELD AVAILABILITY: AB; GI; DCN
 MANUAL CODES: CPI: B07-D13

L146 ANSWER 95 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN

ACCESSION NUMBER: 1996-105173 [11] WPIX

DOC. NO. NON-CPI: N1996-088188

DOC. NO. CPI: C1996-033181

TITLE: Difunctional polymerisation initiator preparation for anionic polymerisation - by dimerising 1-halogen-3,3-di phenyl propane cpd. to form 1,1,6,6-tetra phenyl hexane cpd., for polymerising monomers for toner resin for low cost.

DERWENT CLASS: A60 A89 E14 G08 S06

INVENTOR(S): FULLER, T J

PATENT ASSIGNEE(S): (XERO) XEROX CORP

COUNTRY COUNT: 1

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
US 5487848	A	19960130	(199611)*		66	C07F001-02	--

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
US 5487848	A	US 1994-279610	19940725

PRIORITY APPLN. INFO: US 1994-279610 19940725

INT. PATENT CLASSIF.:

MAIN: C07F001-02

SECONDARY: C07F001-04; C07F001-06

BASIC ABSTRACT:

US 5487848 A UPAB: 19960315

A process comprises dimerising a 1-halogen-3,3-diphenyl propane cpd. to form a 1,1,6,6-tetraphenyl hexane cpd.

Also claimed are:

(a) a process comprising reacting a 3,3-diphenyl-1-propanol cpd. with a 1-halogen-3,3-diphenyl propane cpd.; (b) a process comprising reacting a 1-halogen-3,3-diphenyl propane cpd. with allyl halogen; (c) a process comprising dimerising a halogen-diaryl propane cpd.; (d) a process comprising reacting a diaryl-propanol cpd. with a halogen-diaryl propane cpd; and (e) a process comprising reacting a halogen-diaryl propane cpd. with allyl halogen.

USE Used as initiators in anionic polymerisation of monomers used as toner resins.

ADVANTAGE The effective initiators are prepared by low cost, simple processes.

PREFERRED MATERIALS The halogen in (I) and the allyl halogen are chlorine. The aryl gps. of the tetra-aryl hexane cpd., the ether cpd. and the diaryl-hexene cpd. opt. contain a substit. R(a). a = 1 - 5; and,

R = 2 - 25 C ether, 1 - 25 C alkoxy or aliphatic hydrocarbon.

Dwg. 0/0

FILE SEGMENT: CPI EPI

FIELD AVAILABILITY: AB; DCN

MANUAL CODES: CPI: A02-A; A10-B01; A12-L05C2; E10-H04; G06-G05

EPI: S06-A04C

L146 ANSWER 96 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN

ACCESSION NUMBER: 1996-078556 [09] WPIX
 DOC. NO. CPI: C1996-026060
 TITLE: Anionic initiator preparation for elastomer for increased rebound articles - by reacting **organo-lithium** cpd. with precursor functionalising agent formed by reacting di isopropenyl benzene with sec. amine, for polymer.
 DERWENT CLASS: A60 E12
 INVENTOR(S): ANTKOWIAK, T A; HALL, J E; LAWSON, D F
 PATENT ASSIGNEE(S): (BRID) BRIDGESTONE CORP
 COUNTRY COUNT: 8
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
EP 693500	A1	19960124	(199609)*	EN	13	C08F004-48	
R: DE ES FR GB IT							
JP 08048708	A	19960220	(199617)		11	C08F004-48	
CA 2153945	A	19960119	(199619)			C07F001-02<--	
US 5567815	A	19961022	(199648)		6	C07D223-04	
EP 693500	B1	19990331	(199917)	EN		C08F004-48	
R: DE ES FR GB IT							
DE 69508670	E	19990506	(199924)			C08F004-48	
ES 2129709	T3	19990616	(199930)			C08F004-48	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
EP 693500	A1	EP 1995-110370	19950703
JP 08048708	A	JP 1995-200392	19950713
CA 2153945	A	CA 1995-2153945	19950714
US 5567815	A	US 1994-276363	19940718
EP 693500	B1	EP 1995-110370	19950703
DE 69508670	E	DE 1995-608670	19950703
		EP 1995-110370	19950703
ES 2129709	T3	EP 1995-110370	19950703

FILING DETAILS:

PATENT NO	KIND	PATENT NO
DE 69508670	E Based on	EP 693500
ES 2129709	T3 Based on	EP 693500

PRIORITY APPLN. INFO: US 1994-276363 19940718
 REFERENCE PATENTS: EP 594107; US 3903168; US 5153159
 INT. PATENT CLASSIF.:

MAIN: C07D223-04; C07F001-02; C08F004-48
 SECONDARY: C07D295-04

BASIC ABSTRACT:

EP 693500 A UPAB: 19960305
 Preparation of an anionic initiator comprises reacting:
 1) an **organolithium** cpds. with
 2) a precursor functionalising agent formed by reacting:
 a) a diisopropenyl benzene of formula (I), with
 b) a sec. amine having a hydrogen substit. and otherwise being essentially free of **lithium**-reactive or alkylene reactive substituents.
 Two of Ra-Rf radicals = isopropenyl; and

the remaining Ra-Rf radicals = H, alkyl and cycloalkyl containing 1-6C atoms.

Also claimed is an anionic initiator of formula (II):

R' and R'' = alkyl, cycloalkyl, aryl, alkoxy, alkylalkoxy and arylalkyl substituents, or

R' and R'' are linked together to form heterocyclic ring radical essentially free of substituents or unsubstituted ring atoms that are reactive with lithium or alkylene groups; and

R = alkyl, cycloalkyl, alkenyl, alkynyl, aryl and aralkyl having 1-20 C atoms and short chain length low mol. weight polymers from diolefin and vinyl aryl monomers having up to 25 units.

USE - The anionic initiator can be used to form polymer and copolymer elastomers which can then be used for tyres, power belts etc.

ADVANTAGE - Articles prepared from these (co)polymers show increased rebound, decreased rolling resistance and less heat build-up during mechanical stress operation. Polymer chains are produced at increased rates. The initiator is stable under semi batch and continuous polymerisation operations. Vulcanisable elastomeric compounds are produced having reduced hysteresis at raised temps.

Dwg.0/0

FILE SEGMENT: CPI
FIELD AVAILABILITY: AB; GI; DCN
MANUAL CODES: CPI: A02-A07B; E05-A
ABEQ US 5567815 A UPAB: 19961202

A method of preparing an anionic initiator by reacting:

(1) an organolithium compound with (2) a precursor functionalising agent formed by reacting (a) a diisopropenyl benzene of formula (I), wherein two of the Ra-Rf radicals are isopropenyl and the remaining Ra-Rf radicals are independently selected from the group consisting of hydrogen, alkyl and cycloalkyl containing 1 to 6 carbon atoms, with (b) a secondary amine having the structural formula (II), wherein R' and R'' are the same or different and are selected from the group consisting of C1-20 alkyl groups, C4-20 cycloalkyl groups, aryl groups, alkoxy groups, alkoxyalkyl and arylalkyl groups, or R' and R'' are linked to form -(CH₂)_p- wherein p is an integer from 3 to 20, or said secondary amine is a heterocyclic ring compound selected from the group consisting of: piperidine, pyrrolidine, hexamethyleneimine, dodecamethyleneimine, morpholine, thiomorpholine, N-methyl-piperazine, N-aryl-piperazine, 1-(2-pyridyl)-piperazine, pyrrole, 3-pyrroline, pyrazole, imidazole, indole, indoline and purine.

Dwg.0/0

L146 ANSWER 97 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
ACCESSION NUMBER: 1990-269647 [36] WPIX
DOC. NO. CPI: C1990-116587
TITLE: New amino-chromane and tetra hydro-naphthalene derivs. - useful as 5-hydroxy tryptamine 1A agonists for treating e.g. anxiety and depression.
DERWENT CLASS: B02 B05
INVENTOR(S): FLAUGH, M E; SCHAUS, J M; TITUS, R D
PATENT ASSIGNEE(S): (ELIL) LILLY & CO ELI
COUNTRY COUNT: 27
PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
EP 385658	A	19900905	(199036)*		33		
R: AT BE CH DE ES FR GB GR IT LI LU NL SE							
PT 93218	A	19900831	(199043)				
CA 2010542	A	19900827	(199046)				

HU 53354	T	19901029	(199049)	
AU 9050144	A	19901025	(199050)	
JP 02268151	A	19901101	(199050)	
CN 1045099	A	19900905	(199121)	
ZA 9001277	A	19911030	(199148)	
HU 65268	T	19940530	(199425)	C07C211-42
HU 209481	B	19940628	(199429)	C07C317-32
SU 1826966	A3	19930707	(199501)	13 C07C211-42
EP 385658	B1	19941228	(199505)	EN 51 C07C323-31
R: AT BE CH DE DK ES FR GB GR IT LI LU NL SE				
DE 69015384	E	19950209	(199511)	C07C323-31
ES 2065478	T3	19950216	(199513)	C07C323-31
IE 65769	B	19951115	(199605)	A61K031-135
IL 93464	A	19961016	(199648)	C07C317-34
IL 114715	A	19970110	(199715)	C07D311-12
PH 27444	A	19930702	(199721)	C07C323-31
IL 109647	A	19970415	(199726)	C07C211-59
US 5637624	A	19970610	(199729)	15 A61K031-135
CN 1120532	A	19960417	(199745)	C07C211-58
JP 2954255	B2	19990927	(199945)	20 C07C317-34
JP 11315063	A	19991116	(200005)	19 C07C317-36
JP 3000016	B2	20000117	(200008)	18 C07C317-36
CA 2362972	A1	19900827	(200216)	EN C07D333-46
MX 200801	B	20010208	(200224)	C07C015-24
CA 2010542	C	20020514	(200240)	EN C07C323-38
HU 221625	B1	20021228	(200308)	C07C211-42

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
EP 385658	A	EP 1990-301901	19900222
JP 02268151	A	JP 1990-44308	19900223
ZA 9001277	A	ZA 1990-1277	19900220
HU 65268	T	HU 1992-2449	19900226
HU 209481	B	HU 1990-1048	19900226
SU 1826966	A3	SU 1990-4743297	19900226
EP 385658	B1	EP 1990-301901	19900222
DE 69015384	E	DE 1990-615384	19900222
		EP 1990-301901	19900222
ES 2065478	T3	EP 1990-301901	19900222
IE 65769	B	IE 1990-684	19900226
IL 93464	A	IL 1990-93464	19900220
IL 114715	A	IL 1990-114715	19900220
PH 27444	A	PH 1990-40083	19900222
IL 109647	A	IL 1990-109647	19900220
US 5637624	A Cont of	US 1989-315752	19890227
	Cont of	US 1991-739597	19910729
		US 1993-28642	19930309
CN 1120532	A Div ex	CN 1990-100962	19900226
		CN 1995-106177	19900226
JP 2954255	B2	JP 1990-44308	19900223
JP 11315063	A Div ex	JP 1990-44308	19900223
		JP 1999-5156	19900223
JP 3000016	B2 Div ex	JP 1990-44308	19900223
		JP 1999-5156	19900223
CA 2362972	A1 Div ex	CA 1990-2010542	19900221
		CA 1990-2362972	19900221
MX 200801	B	MX 1995-1209	19950306
CA 2010542	C	CA 1990-2010542	19900221

HU 221625	B1 Div ex	HU 1990-1048	19900226
		HU 1992-2449	19900226

FILING DETAILS:

PATENT NO	KIND	PATENT NO
HU 209481	B Previous Publ.	HU 53354
DE 69015384	E Based on	EP 385658
ES 2065478	T3 Based on	EP 385658
IL 114715	A Div ex	IL 109647
IL 109647	A Div ex	IL 93464
JP 2954255	B2 Previous Publ.	JP 02268151
JP 3000016	B2 Previous Publ.	JP 11315063
HU 221625	B1 Previous Publ.	HU 65268

PRIORITY APPLN. INFO: US 1989-315752 19890227; US
 1991-739597 19910729; US
 1993-28642 19930309

REFERENCE PATENTS: 2.Jnl.Ref; EP 272534; EP 279150; EP 41488; EP 52932;
 01Jnl.Ref

INT. PATENT CLASSIF.: A01N031-13; A61K031-13; C07C013-48; C07C211-42;
 C07C317-32; C07C321-24; C07C321-28; C07C323-31;
 C07D213-70; C07D311-58; C07F001-02

MAIN: A61K031-135; C07C015-24; C07C211-42; C07C211-58;
 C07C211-59; C07C317-32; C07C317-34; C07C317-36;
 C07C323-31; C07C323-38; C07D311-12; C07D333-46

SECONDARY: A01N031-13; A61K031-00; A61K031-10; A61K031-13;
 A61K031-35; A61K031-38; A61K031-40; A61K031-44;
 A61K031-445; A61P043-00; C07B053-00; C07C013-48;
 C07C039-10; C07C209-24; C07C211-29; C07C225-20;
 C07C311-58; C07C321-24; C07C321-28; C07D213-70;
 C07D213-89; C07D307-64; C07D311-02; C07D311-50;
 C07D311-58; C07D311-74; C07D333-34; C07D405-12;
 C07D407-12; C07D409-12; C07F001-02

INDEX: C07M007:00

BASIC ABSTRACT:

EP 385658 A UPAB: 19930928

Amine derivs. of formula (I) and their pharmaceutically acceptable acid addition salts are new. R = 1-4C alkyl, allyl or cyclopropylmethyl; R1 = H, 1-4C alkyl, allyl, cyclopropylmethyl or aryl-(1-4C)alkyl; R2 = H or Me; X = CH2 or O; R3 = 1-8C alkyl, opt. substd. aryl; aryl-(1-4C)alkyl (opt. substd.) or 5-7C cycloalkyl; n = 0-2.

Preparation of optically active 2-amino-1,2,3,4-tetrahydronaphthalene or 3-aminochromane comprises reacting the corresp. 2-tetralone or 3-chromanone with an optically active p-nitro-phenethylamine; separating the resulting 2-(alpha-methyl-p-nitrobenzyl) aminotetralin or 3-(alpha-methyl-p-nitrobenzyl) aminochromane into their optical isomers; and cleaving the p-nitrophenethyl gp. to give an optically active prod.

USE - (I) have high binding affinity to 5-HT1A (5-hydroxytryptamine 1A) receptors. Thus as (I) have 5-HT1A agonist activity, they are useful for treating e.g. sexual dysfunction, anxiety, depression, alcoholism, eating disorders (e.g. anorexia), pain, senile dementia and smoking. Dose is 0.01-20 (pref. 0.05-10, especially 0.1-5)mg/kg/day. Process described in

(B)

can be used to prepare optically active cpds. (I), or intermediates for (I).

0/0

FILE SEGMENT: CPI
 FIELD AVAILABILITY: AB; DCN

MANUAL CODES: CPI: B06-A01; B06-A02; B10-B04B; B12-C06; B12-C10;
B12-D01; B12-G04; B12-J05A; B12-J05B

ABEQ EP 385658 B UPAB: 19950207

A compound of the formula (I) in which R is C1-C4 alkyl, allyl, or cyclopropylmethyl; R1 is hydrogen C1-C4 alkyl, allyl, cyclopropylmethyl, or aryl(C1-C4-alkyl); R2 is hydrogen or methyl; X is -CH2- or -O-; R3 is C1-C8 alkyl, aryl, substituted aryl, aryl(C1-C4-alkyl), substituted aryl(C1-C4 alkyl), or C5-C7 cycloalkyl; n is 0, 1 or 2; and pharmaceutically acceptable acid addition salts thereof.

Dwg.0/0

ABEQ US 5637624 A UPAB: 19970716

A compound of the formula (I), in which R is C1-C4 alkyl, allyl, or cyclopropylmethyl;

R1 is hydrogen, C1-C4 alkyl, allyl, or cyclopropylmethyl;

R2 is hydrogen or methyl;

X is -CH2-;

R3 is C1-C8 alkyl, phenyl, phenyl substituted with C1-C3 alkyl, C1-C3 alkoxy, halo, hydroxy, C1-C3 alkylthio or trifluoromethyl, pyridyl, pyridyl substituted with C1-C3 alkyl, C1-C3 alkoxy, halo, hydroxy, C1-C3 alkylthio or trifluoromethyl, phenyl C1-C4 alkyl, phenyl C1-C4 alkyl substituted on the phenyl ring with C1-C3 alkyl, C1-C3 alkoxy, halo, hydroxy, C1-C3 alkylthio or trifluoromethyl;

n is 0, 1 or 2;

and pharmaceutically acceptable acid addition salts thereof.

Dwg.0/0

L146 ANSWER 98 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN

ACCESSION NUMBER: 1989-305521 [42] WPIX

DOC. NO. CPI: C1989-135459

TITLE: Optically-active 3-phenyl glycidic acid ester cpds. and preparation - useful for preparation of diltiazem

hydrochloride for

coronary vaso-dilation.

DERWENT CLASS: B03

PATENT ASSIGNEE(S): (TANA) TANABE SEIYAKU CO

COUNTRY COUNT: 1

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
JP 01226881	A	19890911	(198942)*		9		
JP 05023264	B	19930402	(199316)		9	C07D301-02	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 01226881	A	JP 1988-52333	19880304
JP 05023264	B	JP 1988-52333	19880304

FILING DETAILS:

PATENT NO	KIND	PATENT NO
JP 05023264	B Based on	JP 01226881

PRIORITY APPLN. INFO: JP 1988-52333 19880304

INT. PATENT CLASSIF.:

MAIN: C07D301-02

SECONDARY: C07B061-00; C07D303-48

ADDITIONAL: C07F001-02

BASIC ABSTRACT:

JP 01226881 A UPAB: 19930923

1. Optically-active trans-3-phenylglycidic acid ester derivs. of formula (I) are produced by treating a halogenoacetic acid ester of formula XCH₂COOR₂ (II) with a benzaldehyde cpd. of formula (III) in the presence of an optically-active lithium amide cpd. and an alkyllithium cpd. of formula (IV) to give a 3-phenylpropionic acid ester derivative of formula (V), and subjecting (V) to intramolecular ring-closing; where R₁ is an ester residue; R₂ is an ester residue; X is a halogen atom; ring A is a phenyl gp. opt. having a substitution gp.; one of R_a and R_b = H and the other = phenyl opt. having a substitution gp.; R_c = a lower alkyl or cycloalkyl gp. and Z = H, lower alkoxy or a N-containing hetero monocyclic gp.

USE/ADVANTAGE - Useful as a material for the synthesis of diltiazem hydrochloride useful as a coronary vasodilator or other various pharmaceuticals.

0/0

FILE SEGMENT: CPI

FIELD AVAILABILITY: AB; DCN

MANUAL CODES: CPI: B07-A03

L146 ANSWER 99 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN

ACCESSION NUMBER: 1989-280011 [39] WPIX

DOC. NO. CPI: C1989-123922

TITLE: 10-Amino indolo isoquinoline derivs. production - from new 2-alkoxy-pyridine cpds. and 2-substd. indole, cyclisation and reaction with amine, used as antitumour and anti-leukaemia agents.

DERWENT CLASS: B02

INVENTOR(S): BOUISSET, M; BOUSQUET, A; DORMOY, J; HEYMES, A; DORMOY, J R

PATENT ASSIGNEE(S): (SNFI) ELF SANOFI; (SNFI) SANOFI SA

COUNTRY COUNT: 17

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
EP 334695	A	19890927	(198939)*	FR	58		
R: AT BE CH DE ES FR GB GR IT LI LU NL SE							
FR 2627493	A	19890825	(198941)				
PT 89775	A	19891004	(198945)				
JP 02111771	A	19900424	(199022)				
US 5079363	A	19920107	(199205)				
CA 1335203	C	19950411	(199522)			C07D471-04	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
EP 334695	A	EP 1989-400500	19890222
FR 2627493	A	FR 1988-2156	19880223
JP 02111771	A	JP 1989-42898	19890222
US 5079363	A	US 1989-313545	19890222
CA 1335203	C	CA 1989-591161	19890215

PRIORITY APPLN. INFO: FR 1988-2156 19880223

REFERENCE PATENTS: EP 10029; FR 2436786

INT. PATENT CLASSIF.: A61K031-47; C07D040-04; C07D209-00; C07D213-64;

C07D213-82; C07D221-00; C07D263-06; C07D401-06;
 C07D413-04; C07D471-04; C07F001-02; C07F003-02;
 C07F005-00; C07F013-00
 MAIN: C07D471-04
 SECONDARY: A61K031-47; C07D040-04; C07D209-00; C07D213-64;
 C07D213-82; C07D221-00; C07D263-06; C07D401-06;
 C07D413-04; C07D471-14; C07F001-02; C07F003-02;
 C07F005-00; C07F013-00

BASIC ABSTRACT:

EP 334695 A UPAB: 19940203

Production of indolo-isoquinoline derivs. of formula (I) and their pharmaceutically acceptable acid addition salts comprise (1) metallising alkoxy pyridine (IIIa); (2) reacting the product (Na) with (aza)indole cpd. (Va) to give hydroxy cpd. (II); (3) cyclising this (opt. after N deprotection) to lactone (VIII); (4) reducing this to cyclic hemiacetal (IX); (5) cyclising this to 10-alkoxy cpd. (X), which (6) is reacted with amine H-Am. In formulae R1 and R1' = H or 1-4C alkyl; X = N or COR2; R2 = 1-4C alkyl or benzyl; Am = amino opt. substd. by -CHR5-(CH2)n-NR3R4; R3, R4 and R5 = H or 1-6C alkyl; n = 1-10; R = 1-4C alkyl; Y = 4,4-dimethyloxaolin-2-yl or CO.NR6R7; R6 and R7 = 1-4C alkyl; Z1 = Li, MgHal, Mnhalo or Ce(halo)2; P = labile protecting gp.; R8 = COR1 or CON(OR7)R6; P' = P or H. Several modifications to the process are claimed.

The 2-alkoxy pyridine cpds. of formula (A) are new; R10 = H, 1-4C alkyl, OH, N(OR7)R6; Z = Z1, -CO-R10 or (Al); W = CO or -C(OH)(R1)-.

USE/ADVANTAGE - (I) are known as antitumour and antileukaemia agents. This process allows them to be prepared on an industrial scale.

Dwg.0/0

FILE SEGMENT: CPI
 FIELD AVAILABILITY: AB; DCN
 MANUAL CODES: CPI: B05-A01B; B05-A03; B06-D01; B06-D05; B06-D18;
 B07-D04; B12-G05; B12-G07

ABEQ US 5079363 A UPAB: 19930923

A new process for mfr. of isoquinoline derivs. of formula (I) comprises metallating (IIIa) into (IVa) and condensing this with (Va), (or similarly condensing (IIIb), with (Vb)) to obt. cpd. (II). (II) is converted to lactone (VIII) then redn. to cyclic hemiacetal (IX) and cyclised to alkoxyisiquinoline (X), which is converted to (I) directly by catalytic reaction with H-Am or indirectly via chloro cpd. (XII).

R and R1 are each 1-4C alkyl; X is either N or C-OR2 with R2 is 1-4C alkyl or benzyl and R5 is H or 1-6C alkyl; n is 1-10; Y is either 4,4-dimethyl-2-oxazolinyl or -C(O)NR6R7 with R6 and R7 each 1-4C alkyl; Z1 is either Li or -MgHal, -MnHal, or -Ce(Hal)2; P is protecting gp.; R8 is -C(O)R1, or formula -C(O)-N(OR7)-R6; R9 is 1-4C alkyl; and M is Li or -MgHal. Am is NH2 opt. substd. by -CH(R5)-(CH2)n-NR3R4.

USE - (I) are antitumour and antileukaemic agents. @@

L146 ANSWER 100 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN

ACCESSION NUMBER: 1986-184541 [29] WPIX

DOC. NO. CPI: C1986-079364

TITLE: Preparation of 2 substd. pyrrolo pyridine(s) - by protecting the 1 nitrogen atom, lithiating the 2 position, and with an electrophilic gp, used is anthelmintics intermediates.

DERWENT CLASS: B02 C02

INVENTOR(S): DORMOY, J R; HEYMES, A; HAYMES, A

PATENT ASSIGNEE(S): (SNFI) SANOFI SA

COUNTRY COUNT: 15

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
EP 187631	A	19860716	(198629)*	FR	32		
R: AT BE CH DE FR GB IT LI LU NL SE							
FR 2574406	A	19860613	(198630)				
JP 61155385	A	19860715	(198634)				
DK 8505768	A	19860613	(198637)				
US 4831144	A	19890516	(198923)				
EP 187631	B	19900905	(199036)				
R: AT BE CH DE FR GB IT LI LU NL SE							
DE 3579577	G	19901011	(199042)				
CA 1299183	C	19920421	(199221)				C07D471-04

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
EP 187631	A	EP 1985-870178	19851211
FR 2574406	A	FR 1984-19029	19841212
JP 61155385	A	JP 1985-280176	19851212
US 4831144	A	US 1988-141508	19880107
CA 1299183	C	CA 1985-497380	19851211

PRIORITY APPLN. INFO: FR 1984-19029 19841212

REFERENCE PATENTS: 1.Jnl.Ref

INT. PATENT CLASSIF.:

MAIN: C07D471-04

SECONDARY: C07D207-32; C07D209-00; C07D213-74; C07D221-00;
C07F001-02; C07F007-08; C07F007-10

BASIC ABSTRACT:

EP 187631 A UPAB: 19930922

Electrophilic groups are attached to the 2-position of a 1H-pyrrolo (3,2-c) pyridine by treating 1H-pyrrolo(3,2-c) pyridine (I) at ambient temperature to 40 deg. C with a halide R-Hal (II), in a solvent with an alkali metal hydroxide and a phase transfer catalyst. The product is an N-protected pyrrolo pyridine (III) R = a labile protecting group Hal = Cl, Br, or I. The prod. (III) is treated with a **lithiating** agent which is either a **lithium** amide or an **alkyl lithium** at -80 to -20 deg. C in the presence of tetramethyl ethylene diamine. The **lithiated** product (IV) is condensed in a solvent at -80 deg. C to ambient temperature with a cpd. capable of replacing the **lithium** with an **electrophilic** group. Z = **electrophilic** group.

Preparation of compounds of formula (V) are also claimed in which R is as defined and Z is H, Li, lower alkyl, -COR₂, -CR₅R₆OH or -Si(R₆)₃
R₂ = H, lower alkyl, -OR₃, or -N(R₄)₂ R₃ = H or lower alkyl R₄ = lower alkyl R₅ = H or lower alkyl R₆ = phenyl or lower alkyl.

USE - Intermediates, especially for biologically active materials such as the anthelmintics.

0/0

FILE SEGMENT: CPI

FIELD AVAILABILITY: AB; DCN

MANUAL CODES: CPI: B05-A01B; B05-B01B; B06-D05; C05-A01B; C05-B01B;
C06-D05; N05-D

ABEQ EP 187631 B UPAB: 19930922

Method of fixing an **electrophilic** gp. in the 2-position of 1H-pyrrolo(3,2-c)pyridine derivs. characterised in that: a) 1H-pyrrolo(3,2-c)pyridine is reacted, at room temp. and in a solvent, with an alkali metal hydroxide and in the presence of an interphase transfer

catalyst then, at a temp. between room temp. and 40 deg C with a halide of general formula: R-Hal in which R represents a methoxymethyl, benzyloxymethyl, benzenesulphonyl, p-toluenesulphonyl or tert. butoxycarbonyl gp. and Hal represents a chlorine, bromine or iodine atom, to obtain the N-protected 1H-pyrrolo(3,2-c) pyridine derivs. of general formula (I) in which R has the same meaning as above. b) the N-protected 1H-pyrrolo(3,2-c)pyridine obtd. in paragraph a) above is reacted in a solvent, at a temp. between -80 deg C and -20 deg C and in the presence of tetramethylethylenediamine, with a lithiation agent which is either a lithium amide or an alkyl lithium, to obtain the 2-lithio derivs. of general formula (II) in which R has the same meaning as above. c) the 2-lithio deriv. obtained in paragraph b) above is condensed in a solvent and at a temp. between -80 deg C and room temp. with a reagent capable of producing an electrophilic gp., to obtain the 1H-pyrrolo(3,2-c)pyridine derivs. of formula I substd. in the 2-position by an electrophilic gp.

ABEQ US 4831144 A UPAB: 19930922

1H-pyrrolo(3,2-c)pyridine deriv of formula (I), where R is protecting gp viz alkoxyalkyl, aralkoxyalkyl, carbalkoxyalkyl, and Z is H or Li, is new. Esp cpds are 1-benzene-sulphonyl -1H-pyrrolo(3,2-c)pyridine and 1-tert-butoxycarbonyl-1H-pyrrolo (3,2-c)pyridine and their 2-litho derivs. These cpds protected at the 1-function, are obtd by new process comprising fixing electrophilic gp in 2-position of the N-protected 1-position cpd by lithiation with Li amide or alkyl Li at -80 to -20 deg.C in presence of tetramethyldiamine, then condensing the 2-litho deriv so obtd with electrophilic gp reagent at -80 deg. C to RT.

USE - Chemical intermediates utilising liability of R10 or substn or modification at 2-position.

L146 ANSWER 101 OF 115 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN

ACCESSION NUMBER: 1982-09553J [51] WPIX

TITLE: 1,3-Benzodiazepine derivs. and their intermediates - 2-phenethyl-tri-methyl-acetanilide derivs., used as antidepressants, analgesics and anticonvulsants.

DERWENT CLASS: B02 B05

INVENTOR(S): LEE, G E; LEE, T B K

PATENT ASSIGNEE(S): (HMRI) HOECHST ROUSSEL PHARM INC; (HMRI) HOECHST ROUSSEL PHARM INC

COUNTRY COUNT: 13

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN	IPC
EP 66773	A	19821215	(198251)*	EN	17		
	R:	AT BE CH DE FR GB IT LI NL SE					
KR 8802290	B	19881022	(198924)				
JP 03052453	B	19910812	(199136)				
JP 04217965	A	19920807	(199238)		4	C07D243-14	
US 5349086	A	19940920	(199437)		5	C07C231-08	
US 5489681	A	19960206	(199612)		5	C07D243-204	

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
EP 66773	A	EP 1982-104546	19820525
JP 03052453	B	JP 1982-88956	19820527
JP 04217965	A Div ex	JP 1982-88956	19820527
		JP 1991-61022	19820527

US 5349086	A	Cont of	US 1981-267990	19810528
		Div ex	US 1985-757765	19850723
		Cont of	US 1987-98210	19870918
		Cont of	US 1989-384115	19890721
		Cont of	US 1990-579262	19900907
		Cont of	US 1991-737610	19910729
		Cont of	US 1992-870772	19920421
			US 1992-980449	19921123
US 5489681	A	Cont of	US 1981-267990	19810528
		Div ex	US 1985-757765	19850723
		Cont of	US 1987-98210	19870918
		Cont of	US 1989-384115	19890721
		Cont of	US 1990-579262	19900907
		Cont of	US 1991-737610	19910729
		Cont of	US 1992-870772	19920421
		Div ex	US 1992-980449	19921123
			US 1994-304662	19940909

FILING DETAILS:

PATENT NO	KIND	PATENT NO
US 5349086	A Div ex	US 4709093
US 5489681	A Div ex	US 4709093
	Div ex	US 5349086

PRIORITY APPLN. INFO: US 1981-267990 19810528; US
 1987-98210 19870918; US
 1989-384115 19890721; US
 1990-579262 19900907; US
 1991-737610 19910729; US
 1992-870772 19920421; US
 1992-980449 19921123; US
 1994-304662 19940909

REFERENCE PATENTS: EP 9800

INT. PATENT CLASSIF.:

MAIN: C07C231-08; C07D243-14; C07D243-204
 SECONDARY: A61K031-55; C07C013-50; C07C087-50; C07C102-00;
 C07C103-44; C07C231-14; C07C233-43; C07D243-04;
 C07F001-02

BASIC ABSTRACT:

EP 66773 A UPAB: 19960417
 N-(2-(2-amino -2-phenylethyl)phenyl)-2,2-dimethyl propionamide derivs. of
 the formula (I) are new (where R₁ is H or (1-5C) alkyl).
 Preparation of 4,5-dihydro-4-phenyl- 3H-1,3-benzodiazepines (VII) and
 their salts by hydrolysis of (I) and cyclising the prod. (V) with
 orthoester (VI) (where R is H or (1-5C) alkyl and R₂ is methyl or ethyl).
 (I) are intermediates for (VII) which are antidepressants, analgesics
 and anticonvulsants.

FILE SEGMENT: CPI

FIELD AVAILABILITY: AB

MANUAL CODES: CPI: B06-D07; B10-B02F; B12-C06; B12-D01; B12-D04

ABEQ EP 66773 B UPAB: 19930915

N-(2-(2-amino 2-phenylethyl) phenyl)2,2-dimethyl propanamides of formula
 (I) are new. R₁ is H or 1-5C alkyl.

They are prepd. e.g. by reacting an N-acylated O-toluidine of formula
 (II) with n-alkyl lithium and reacting this with an
 N-benzylidene amine of formula (III). The reaction is pref. carried out in
 an inert (a) ethereal or (b) hydrocarbon solvent and in an anhydrous
 atmosphere. (a) is pref. diethyl ether, tetrahydrofuran or dimethoxy

ethane. (b) is pref. hexane. The reaction is pref. carried out at -70 to 30, esp. -10 to 30 deg.C. for 0.5 to 5 hrs., esp. 1 to 2 hrs.

USE - As intermediates for 4,5-dihydro-4-phenyl-3H,-1,3 benzodiazepines which are antidepressants, analgesics and anticonvulsants.

ABEQ US 4709093 A UPAB: 19930915

N-(2-(2-Methylamino-2-phenylethyl)phenyl)-2,2-dimethylpropanamide of formula (II) is new. (II) may be prepd. e.g. by reacting an N-acylated o-toluidine (III) with n-alkyl lithium to form dilithio intermediate (IV) which gives (II) by quenching with N-benzylidene methylamine.

USE - Hydrolysis of (II) yields free base or salt which can be cyclised to form 4,5-dihydro-2,3-dimethyl-4-phenyl-3H-1,3-benzodiazepine of formula (I). Useful as antidepressant, analgesic and anticonvulsant. Simple economical high yield prepn.

ABEQ US 5349086 A UPAB: 19941109

Prepn. of N-(2-(2-methylamino-2-phenylethyl)phenyl)-2,2-dimethylpropanamide of formula (II) comprises reacting an N-acylated o-toluidine of formula (III) with n-alkyllithium to provide a dilithio intermediate of formula (IV) and quenching it with N-benzylidenemethylamine. Pref. N-((2-methyl)-phenyl)-2,2-dimethylpropanamide is reacted with n-BuLi in THF and hexane in anhydrous atmos. at -10 to +30 deg C for 1-2 hrs. to form (IV) which is quenched with 1-2 molar equivs. of N-benzylaminemethylamine at 0-25 deg C for 5-60 mins. in anhydrous atmos.

USE - (II) is hydrolysed to free base of formula (V) which can be cyclised to 4,5-dihydro-2,3-dimethyl-4-phenyl-3H-1,3-benzodiazepine of formula (I) which is used as antidepressant, analgesic and anticonvulsant. Dwg.0/0

ABEQ US 5489681 A UPAB: 19960322

A process for preparing 4,5-dihydro-2,3-dimethyl-4-phenyl-3H-1,3-benzodiazepine or a pharmaceutically acceptable salt thereof, comprises (A) reacting N-((2-methyl)phenyl)-2,2-dimethylpropanamide with n-alkyllithium to provide a dilithio intermediate of the formula (I), (B) quenching the dilithio intermediate with N-benzylidenemethylamine to form N-(2-(2-methylamino-2-phenylethyl)phenyl)-2,2-dimethylpropanamide, (C) hydrolysing the N-(2-(2-methylamino-2-phenylmethyl)phenyl)-2,2-dimethylpropanamide to form N-methyl-2-amino-alpha-phenylphenethylamine as a free base or salt thereof, and (D) cyclising said N-methyl-2-amino-alpha-phenylphenethylamine by reaction with a compound of the formula (VI) or (VII) to form 4,5-dihydro-2,3-dimethyl-4-phenyl-3H-1,3-benzodiazepine or a pharmaceutically acceptable salt thereof. Dwg.0/0

=> d ibib ed ab ind 102-115

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, CASREACT, USPATFULL, WPIX, MEDLINE, BIOSIS, SCISEARCH, DISSABS' - CONTINUE? (Y)/N:y

L146 ANSWER 102 OF 115 MEDLINE on STN

ACCESSION NUMBER: 96071178 MEDLINE

DOCUMENT NUMBER: PubMed ID: 7479079

TITLE: Solid-phase synthesis of a nucleopeptide from the linking site of adenovirus-2 nucleoprotein, -Ser(p5'CATCAT)-Gly-Asp-. Convergent versus stepwise strategy.

AUTHOR: Robles J; Pedroso E; Grandas A

CORPORATE SOURCE: Departament de Quimica Organica, Facultat de Quimica, Universitat de Barcelona, Barcelona, Spain.

SOURCE: Nucleic acids research, (1995 Oct 25) Vol. 23, No. 20, pp. 4151-61.
Journal code: 0411011. ISSN: 0305-1048.
PUB. COUNTRY: ENGLAND: United Kingdom
DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)
LANGUAGE: English
FILE SEGMENT: Priority Journals
ENTRY MONTH: 199512
ENTRY DATE: Entered STN: 24 Jan 1996
Last Updated on STN: 24 Jan 1996
Entered Medline: 21 Dec 1995

ED Entered STN: 24 Jan 1996
Last Updated on STN: 24 Jan 1996
Entered Medline: 21 Dec 1995
AB The synthesis of a nucleopeptide with the sequence -Ser(p5'CATCAT)-Gly-Asp- has been undertaken by either convergent or stepwise solid-phase strategies, both of which use base-labile permanent protecting groups. The **coupling** of phosphitylated protected peptides onto oligonucleotide-resins did not afford the desired nucleopeptide, which was nevertheless obtained after oligonucleotide elongation at the hydroxyl group of the resin-bound peptide and deprotection under mild basic conditions. A preliminary study on the stability of different nucleopeptides to bases is also reported.
CT Adenoviruses, Human: CH, chemistry
Amino Acid Sequence
Ammonia: PD, pharmacology
Carbonates: PD, pharmacology
Comparative Study
*Deoxyribonucleoproteins: CS, chemical synthesis
Deoxyribonucleoproteins: DE, drug effects
Lithium Compounds: PD, pharmacology
Molecular Sequence Data
*Oligodeoxyribonucleotides: CS, chemical synthesis
Potassium: PD, pharmacology
Research Support, Non-U.S. Gov't
Serine: CH, chemistry
Viral Proteins: CH, chemistry
RN 1310-65-2 (lithium hydroxide); 56-45-1 (Serine); 584-08-7 (potassium carbonate); 7440-09-7 (Potassium); 7664-41-7 (Ammonia)
CN 0 (Carbonates); 0 (Deoxyribonucleoproteins); 0 (Lithium Compounds); 0 (Oligodeoxyribonucleotides); 0 (Viral Proteins)

L146 ANSWER 103 OF 115 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on STN DUPLICATE 48

ACCESSION NUMBER: 1993:121771 BIOSIS
DOCUMENT NUMBER: PREV199395065871
TITLE: Naphthalene-catalysed lithiation of functionalized chloroarenes: Regioselective preparation and reactivity of functionalized lithioarenes.
AUTHOR(S): Guijarro, Albert; Ramon, Diego J.; Yus, Miguel [Reprint author]
CORPORATE SOURCE: Dep. Quim. Org., Fac. Ciencias, Univ. Alicante, Apdo. 99, 03080 Alicante, Spain
SOURCE: Tetrahedron, (1993) Vol. 49, No. 2, pp. 469-482.
CODEN: TETRAB. ISSN: 0040-4020.
DOCUMENT TYPE: Article
LANGUAGE: English
ENTRY DATE: Entered STN: 27 Feb 1993
Last Updated on STN: 27 Feb 1993
ED Entered STN: 27 Feb 1993

Last Updated on STN: 27 Feb 1993

AB The lithiation of different functionalized chloroarenes (dichlorobenzenes 1 and 3, mono and dichlorophenols 9 and 14, and chloropivalanilides 18) in the presence of a catalytic amount of naphthalene leads to the corresponding functionalized lithioarenes, which react with **electrophiles** to give the expected polyfunctionalized aromatic molecules 2, 4, 10, 19, 21, 22 and 24 in a regioselective manner. In the case of the starting from chlorinated phenols or anilides a **deprotonation** of the functional group is carried out prior to the **lithiation** process; only for 2-chloropivalanilide 18o a **coupling** reaction leading to 2-n-butylpivalanilide is observed when an excess of n-butyllithium is used in the **deprotonation** step.

CC Biochemistry methods - General 10050
Biochemistry studies - General 10060
Pharmacology - General 22002

IT Major Concepts

Biochemistry and Molecular Biophysics; Pharmacology

IT Miscellaneous Descriptors

PHARMACEUTICAL RELEVANCE; SYNTHETIC METHOD

L146 ANSWER 104 OF 115 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on STN

ACCESSION NUMBER: 2006:343709 BIOSIS

DOCUMENT NUMBER: PREV200600342841

TITLE: Synthesis and applications of arginine mimetics.

AUTHOR(S): Smith, Alfred Gordon [Reprint Author]

CORPORATE SOURCE: Univ Delaware, Newark, DE 19717 USA

SOURCE: FASEB Journal, (MAR 6 2006) Vol. 20, No. 4, Part 1, pp. A67.

Meeting Info.: Experimental Biology 2006 Meeting. San Francisco, CA, USA. April 01 -05, 2006. Amer Assoc Anatomists; Amer Physiol Soc; Amer Soc Biochem & Mol Biol; Amer Soc Investigat Pathol; Amer Soc Nutr; Amer Soc Pharmacol & Expt Therapeut.

CODEN: FAJOEC. ISSN: 0892-6638.

DOCUMENT TYPE: Conference; (Meeting)

Conference; Abstract; (Meeting Abstract)

LANGUAGE: English

ENTRY DATE: Entered STN: 12 Jul 2006

Last Updated on STN: 12 Jul 2006

ED Entered STN: 12 Jul 2006

Last Updated on STN: 12 Jul 2006

AB Protein-protein, protein-RNA, and protein-DNA interactions are broadly mediated through the guanidinium functionality of arginine residues. However, specific recognition by arginine is limited, because the guanidinium functionality is attached to a linear alkyl group. To achieve specific molecular recognition, arginine mimetics are used, which place functional groups adjacent to a guanidinium. In order to specifically target arginine-mediated recognition, we developed convenient syntheses of alpha- guanidino acids, in which the amine of an amino acid is converted into a guanidinium. The alpha-substituted guanidiniums of guanidino acids and the side chain of the amino acid work synergistically toward molecular recognition with greater affinity for the target site. We have designed arginine mimetics for specific and high affinity molecular recognition by **coupling** protected guanidino acids to alcohol and amine nucleophiles. Protected guanidino acids of Gly, Phe, Val, and Leu were readily synthesized from methyl esters of alpha-amino acids by guanylation of the amine with bis-boc-thiourea and Mukaiyama's reagent. Protected guanidino acids, with a free carboxylic acid for **coupling** to

nucleophiles, were generated by saponification of the methyl ester using LiOH. Arginine mimetics were synthesized by **coupling** protected guanidino acids to hydroxyl and amino groups to generate complex alpha-substituted guanidiniums. Molecules containing alpha-guanidino acids were applied to specific protein and RNA recognition.

CC General biology - Symposia, transactions and proceedings 00520
 Biochemistry studies - General 10060
 Biochemistry studies - Nucleic acids, purines and pyrimidines 10062
 IT Major Concepts
 Biochemistry and Molecular Biophysics
 IT Chemicals & Biochemicals
 methyl esters; RNA; alcohol; guanidinium; alkyl; protein-protein interactions; alpha-amino acids; amine nucleophiles; lithium hydroxide; protein-DNA interactions; protein-RNA interactions; alpha-guanidino acids; bis-boc-thiourea; arginine mimetics; Mukaiyama's reagent
 IT Miscellaneous Descriptors
 molecular recognition
 ORGN Classifier
 Organisms 00500
 Super Taxa
 Organisms
 Organism Name
 organism (common)
 Taxa Notes
 Organisms
 RN 64-17-5 (alcohol)
 25215-10-5 (guanidinium)
 1310-65-2 (lithium hydroxide)

L146 ANSWER 105 OF 115 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on STN

ACCESSION NUMBER: 2005:561237 BIOSIS
 DOCUMENT NUMBER: PREV200510348397
 TITLE: Scope and limitations of the catalytic asymmetric rearrangement of epoxides to allylic alcohols using chiral lithium amide bases/**lithiated** imidazoles.
 AUTHOR(S): Oxenford, Sally J.; Wright, Jonathan M.; O'Brien, Peter [Reprint Author]; Panday, Narendra; Shipton, Mark R.
 CORPORATE SOURCE: Univ York, Dept Chem, York YO10 5DD, N Yorkshire, UK paobl@york.ac.uk
 SOURCE: Tetrahedron Letters, (NOV 28 2005) Vol. 46, No. 48, pp. 8315-8318.
 CODEN: TELEAY. ISSN: 0040-4039.
 DOCUMENT TYPE: Article
 LANGUAGE: English
 ENTRY DATE: Entered STN: 7 Dec 2005
 Last Updated on STN: 7 Dec 2005

ED Entered STN: 7 Dec 2005

Last Updated on STN: 7 Dec 2005

AB The catalytic asymmetric rearrangement of functionalised cyclohexene and cyclopentene oxides has been studied using sub-stoichiometric amounts of a chiral lithium amide in combination with a stoichiometric amount of three different **lithiated** imidazoles. I-Methylimidazole that had been **lithiated** at the C-2 aryl position gave the highest enantioselectivity (82% ee). With 1,2-dimethylimidazole that had been **lithiated** at the C-2 methyl group, epoxide ring opening occurred as an unexpected and competing process. Ultimately, ring opening was suppressed using a more sterically hindered imidazole. In all catalytic examples, a racemic background reaction (presumably due to rearrangement by the **lithiated** imidazoles) was observed. (c) 2005 Elsevier

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CC Pathology - Therapy 12512
Pharmacology - General 22002

IT Major Concepts
Pharmaceuticals (Pharmacology)

IT Chemicals & Biochemicals
cyclohexene; 1-methylimidazole; cyclopentene oxide; lithium amide:
asymmetric **deprotonation**; 1,2-dimethylimidazole

RN 110-83-8 (cyclohexene)
616-47-7 (1-methylimidazole)
285-67-6 (cyclopentene oxide)
7782-89-0 (lithium amide)

L146 ANSWER 106 OF 115 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on
STN

ACCESSION NUMBER: 2004:304222 BIOSIS

DOCUMENT NUMBER: PREV200400306859

TITLE: Asymmetric synthesis of axially chiral benzamides and
anilides utilizing planar chiral arene chromium complexes.

AUTHOR(S): Koide, Hiroshige; Hata, Takeshi; Yoshihara, Kohei;
Kamikawa, Ken; Uemura, Motokazu [Reprint Author]

CORPORATE SOURCE: Fac Integrated Arts and SciDept Chem, Univ Osaka
Prefecture, Sakai, Osaka, 5998531, Japan
uemura@ms.cias.osakafu-u.ac.jp

SOURCE: Tetrahedron, (May 10 2004) Vol. 60, No. 20, pp. 4527-4541.
print.
ISSN: 0040-4020 (ISSN print).

DOCUMENT TYPE: Article

LANGUAGE: English

ENTRY DATE: Entered STN: 7 Jul 2004

Last Updated on STN: 7 Jul 2004

ED Entered STN: 7 Jul 2004

Last Updated on STN: 7 Jul 2004

AB Optically active axially chiral 2,6-disubstituted benzamides and anilides
were stereoselectively prepared by utilizing planar chiral (arene)chromium
complexes. Nucleophilic addition to enantiomerically pure planar chiral
tricarbonyl(N,N-diethyl-2-methyl-6-formyl- (or 6-acyl)benzamide)chromium
complex gave axially chiral 2-methyl-6-substituted N,N-diethyl benzamide
chromium complexes with high selectivity. An alternative method for the
preparation of axial chiral benzamides or anilides is an enantiotopic
lithiation at the benzylic methyl of prochiral tricarbonylchromium
complexes of N,N-diethyl-2,6-dimethylbenzamide and N-methyl-N-acyl-2,6-
dimethylaniline with a chiral lithium amide followed by
electrophilic substitution. The resulting axially chiral
chromium-complexed benzamides and anilides were oxidized in air to give
chromium-free axially chiral benzamides and anilides in enantiomerically
enriched form without axial bond rotation at room temperature. Copyright
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CC Biochemistry studies - General 10060

IT Major Concepts
Biochemistry and Molecular Biophysics; Methods and Techniques

IT Chemicals & Biochemicals
(tricarbonyl(N,N-diethyl-2-methyl-6-acyl)benzamide)chromium complex:
enantiomerically pure, planar chiral; (tricarbonyl(N,N-diethyl-2-methyl-
6-formyl-benzamide)chromium complex: enantiomerically pure, planar
chiral; 2-methyl-6-substituted N,N-diethyl benzamide chromium
complexes: axially chiral; N,N-diethyl-2,6-dimethylbenzamide prochiral
tricarbonylchromium complexes; N-methyl-N-acyl-2,6-dimethylaniline
[prochiral tricarbonylchromium complexes]; axially chiral
2,6-disubstituted benzamides: asymmetric synthesis, optically active;

axially chiral anilides: asymmetric synthesis; lithium amide: chiral;
planar chiral arene chromium complexes

IT Methods & Equipment
 electrophilic substitution: laboratory techniques;
 enantiotopic **lithiation**: laboratory techniques; nucleophilic
 addition: laboratory techniques

IT Miscellaneous Descriptors
 room temperature; selectivity

RN 55-21-0D (axially chiral 2,6-disubstituted benzamides)
 7782-89-0 (lithium amide)

L146 ANSWER 107 OF 115 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on
STN

ACCESSION NUMBER: 2004:226373 BIOSIS

DOCUMENT NUMBER: PREV200400226791

TITLE: Asymmetric reactions based on activation and structure
control of molecule: Asymmetric reaction of
lithiated nucleophiles.

AUTHOR(S): Tomioka, Kiyoshi [Reprint Author]

CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, Kyoto
University, Yoshida, Sakyo-ku, Kyoto, 606-8501, Japan
tomioka@pharm.kyoto-u.ac.jp

SOURCE: Yakugaku Zasshi, (February 2004) Vol. 124, No. 2, pp.
43-53. print.
ISSN: 0031-6903 (ISSN print).

DOCUMENT TYPE: Article

LANGUAGE: Japanese

ENTRY DATE: Entered STN: 21 Apr 2004

Last Updated on STN: 21 Apr 2004

ED Entered STN: 21 Apr 2004

Last Updated on STN: 21 Apr 2004

AB The methodology we developed relies on an external chiral coordinating
reagent that forms a deaggregated chelate complex with organolithium
reagents. Under the positive control of a chiral dimethyl ether of
stilbenediol 4, an asymmetric conjugate addition reaction of organolithium
reagents with unsaturated imines and esters proceeded successfully to
yield the corresponding addition products with reasonably high
stereoselectivity. The sense of stereochemistry is predictable based on a
coordination model. The methodology has been extended to a catalytic
asymmetric 1,2-addition reaction of organolithium reagents with imines.
An enantiotopic group differentiating the opening of cyclohexene oxide
with organolithium was also mediated by a chiral ligand. The asymmetric
Horner-Wadsworth-Emmons reaction of phosphonates and Peterson reaction of
alpha-silyl ester with 4-substituted cyclohexanone were another successful
extension of the methodology. A three-component reagent of lithium ester
enolate, lithium amide, and chiral diether reacts with imines to afford
beta-lactam with reasonably high enantioselectivity. Tridentate
aminoether ligands were also shown to affect the catalytic asymmetric
addition of lithium ester enolates to imines, giving, beta-lactams with
high enantioselectivity. Asymmetric conjugate addition of lithium amide
to enolates was mediated by a chiral diether ligand to give the
beta-aminoester with high yield and enantioselectivity. The methodology
has been successfully applied to an asymmetric synthesis of biologically
potent compounds. Dihydropyridine, a promising anti-Parkinsonism candidate,
and salsolidine, a representative isoquinoline alkaloid, have been
synthesized using asymmetric addition reactions of organolithium reagents
as the key steps.

CC Biochemistry studies - General 10060

IT Major Concepts

Biochemistry and Molecular Biophysics; Methods and Techniques

IT Chemicals & Biochemicals
4-substituted cyclohexanone; alpha-silylester; beta-lactam; chiral diether; cyclohexene oxide; lithiated nucleophiles; lithium amide; lithium ester enolate; organolithium reagents; phosphonates; stilbenediol; tridentate aminoether ligands

IT Methods & Equipment
Peterson reaction: laboratory techniques; addition reaction: laboratory techniques; asymmetric Horner-Wadsworth-Emmons reaction: laboratory techniques

RN 108-94-1D (4-substituted cyclohexanone)
286-20-4 (cyclohexene oxide)
7782-89-0 (lithium amide)
15477-76-6 (phosphonates)
29718-22-7 (stilbenediol)

L146 ANSWER 108 OF 115 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on STN

ACCESSION NUMBER: 1991:337303 BIOSIS
DOCUMENT NUMBER: PREV199192036678; BA92:36678
TITLE: AN ENANTIOSELECTIVE DEPROTONATION ROUTE TO A VERSATILE INTERMEDIATE FOR C NUCLEOSIDE SYNTHESIS.
AUTHOR(S): COX P J [Reprint author]; SIMPKINS N S
CORPORATE SOURCE: DEP CHEM, UNIV NOTTINGHAM, UNIVERSITY PARK, NOTTINGHAM NG7 2RD, UK
SOURCE: Synlett, (1991) No. 5, pp. 321-323.
CODEN: SYNLES. ISSN: 0936-5214.
DOCUMENT TYPE: Article
FILE SEGMENT: BA
LANGUAGE: ENGLISH
ENTRY DATE: Entered STN: 31 Jul 1991
Last Updated on STN: 11 Sep 1991

ED Entered STN: 31 Jul 1991
Last Updated on STN: 11 Sep 1991

AB The asymmetric transformation of ketone 1 (exo-cis-6,7-isopropylidenedioxy-8-oxabicyclo[3.2.1]octan-3-one) into optically active silyl enol ether 2 (exo-cis-6,7-isopropylidenedioxy-3-trimethylsiloxy-8-oxabicyclo[3.2.1]oct-2-ene) in up to 85% ee was achieved using the homochiral lithium amide base 6 [lithium (R,R)-bis(1-phenylethyl)amide]. Conversion of 2 into a known key intermediate 3 (methyl 2,3-O-isopropylidene-β-ribofuranosyl-acetate) for C-nucleoside synthesis was possible in a highly efficient two-step sequence.

CC Biochemistry methods - Nucleic acids, purines and pyrimidines 10052
Biochemistry studies - General 10060
Biochemistry studies - Nucleic acids, purines and pyrimidines 10062
Biochemistry studies - Minerals 10069
Biophysics - Molecular properties and macromolecules 10506

IT Major Concepts
Biochemistry and Molecular Biophysics

IT Miscellaneous Descriptors
KETONE SILYL ENOL ETHER LITHIUM AMIDE BASE

RN 13765-44-1 (SILYL)
7782-89-0 (LITHIUM AMIDE)

L146 ANSWER 109 OF 115 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on STN

ACCESSION NUMBER: 1991:234588 BIOSIS
DOCUMENT NUMBER: PREV199140108753; BR40:108753
TITLE: ASYMMETRIC SYNTHESIS USING HOMOCHIRAL LITHIUM AMIDE BASES.
AUTHOR(S): COX P J [Reprint author]; SIMPKINS N S
CORPORATE SOURCE: DEP CHEM, UNIV NOTTINGHAM, UNIVERSITY PARK, NOTTINGHAM NG7

2RD, UK
SOURCE: Tetrahedron Asymmetry, (1991) Vol. 2, No. 1, pp. 1-26.
CODEN: TASYE3. ISSN: 0957-4166.

DOCUMENT TYPE: Article

FILE SEGMENT: BR

LANGUAGE: ENGLISH

ENTRY DATE: Entered STN: 21 May 1991

Last Updated on STN: 16 Jul 1991

ED Entered STN: 21 May 1991

Last Updated on STN: 16 Jul 1991

CC Biochemistry methods - General 10050

Biochemistry methods - Minerals 10059

Biochemistry studies - General 10060

Biochemistry studies - Minerals 10069

IT Major Concepts

Biochemistry and Molecular Biophysics

IT Miscellaneous Descriptors

REVIEW **DEPROTONATION** CHIRAL AUXILIARIES

RN 7782-89-0 (LITHIUM AMIDE)

L146 ANSWER 110 OF 115 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on
STN

ACCESSION NUMBER: 1986:187307 BIOSIS

DOCUMENT NUMBER: PREV198630099179; BR30:99179

TITLE: ENANTIOSELECTIVE **DEPROTONATION** BY CHIRAL LITHIUM
AMIDE BASES ASYMMETRIC SYNTHESIS OF TRIMETHYLSILYL-ENOL
ETHERS FROM 4 ALKYL CYCLOHEXANONES.

AUTHOR(S): SHIRAI R [Reprint author]; TANAKA M; KOGA K

CORPORATE SOURCE: FACULTY OF PHARMACEUTICAL SCIENCES, UNIVERSITY OF TOKYO,
HONGO, BUNKYO-KU, TOKYO 113, JAPAN

SOURCE: Journal of the American Chemical Society, (1986) Vol. 108,
No. 3, pp. 543-545.

CODEN: JACSAT. ISSN: 0002-7863:

DOCUMENT TYPE: Article

FILE SEGMENT: BR

LANGUAGE: ENGLISH

ENTRY DATE: Entered STN: 22 May 1986

Last Updated on STN: 22 May 1986

ED Entered STN: 22 May 1986

Last Updated on STN: 22 May 1986

CC Biochemistry methods - Minerals 10059

Biochemistry studies - Minerals 10069

Biophysics - Methods and techniques 10504

Biophysics - Molecular properties and macromolecules 10506

IT Major Concepts

Biochemistry and Molecular Biophysics

IT Miscellaneous Descriptors

COLUMN CHROMATOGRAPHY

RN 7782-89-0 (LITHIUM AMIDE)

L146 ANSWER 111 OF 115 BIOSIS COPYRIGHT (c) 2006 The Thomson Corporation on
STN

ACCESSION NUMBER: 1980:219176 BIOSIS

DOCUMENT NUMBER: PREV198070011672; BA70:11672

TITLE: NEW METHODOLOGY FOR THE INTRODUCTION OF SULFUR INTO ORGANIC
MOLECULES SYNTHESIS OF ANHYDROUS LITHIUM SULFIDE LITHIUM DI
SULFIDE AND LITHIUM ORGANO DI SULFIDE SPECIES BY LITHIUM
TRI ETHYL BOROHYDRIDE REDUCTION OF ELEMENTAL SULFUR AND DI
SULFIDES.

AUTHOR(S): GLADYSZ J A [Reprint author]; WONG V K; JICK B S

CORPORATE SOURCE: DEP CHEM, UNIV CALIF, LOS ANGELES, CALIF 90024, USA
 SOURCE: Tetrahedron, (1979) Vol. 35, No. 20, pp. 2329-2336.
 CODEN: TETRAB. ISSN: 0040-4020.

DOCUMENT TYPE: Article
 FILE SEGMENT: BA
 LANGUAGE: ENGLISH

AB Anhydrous THF [tetrahydrofuran] solutions of Li₂S or Li₂S₂ (or chemically equivalent species) are rapidly and quantitatively formed by the reaction of common yellow S with appropriate stoichiometries of commercially available LiEt₃BH [lithium triethylborohydride]. Only volatile by-products H₂ and Et₃B [ethylboride] are produced; but the Et₃B probably associates with the anionic S species generated. Subsequent reaction with electrophiles (alkylating agents or acylating agents) affords sulfide or disulfide derivatives in high yields. Disulfides are cleaved to lithium mercaptides by LiEt₃BH. Subsequent addition of electrophiles affords unsymmetrical sulfides. Trisulfides and tetrasulfides can also be prepared by LiEt₃BH reduction of S₈, but only in low yield.

CC Comparative biochemistry 10010
 Biochemistry methods - General 10050
 Biochemistry methods - Minerals 10059
 Biochemistry studies - General 10060
 Biochemistry studies - Minerals 10069
 Biophysics - Methods and techniques 10504
 Biophysics - Molecular properties and macromolecules 10506
 Movement 12100
 Pharmacology - General 22002
 IT Major Concepts
 Biochemistry and Molecular Biophysics; Pharmacology
 RN 7704-34-9 (SULFUR)
 51148-09-5 (LITHIUM DISULFIDE)
 7439-93-2 (LITHIUM)
 22560-16-3 (LITHIUM TRIETHYLBOROHYDRIDE)
 16734-12-6 (DISULFIDES)

L146 ANSWER 112 OF 115 SCISEARCH COPYRIGHT (c) 2006 The Thomson Corporation on STN

ACCESSION NUMBER: 1995:721713 SCISEARCH

THE GENUINE ARTICLE: RZ313

TITLE: HYDROCARBON-BRIDGED COMPLEXES .33. SYNTHESIS OF DINUCLEAR HYDROCARBON-BRIDGED COMPLEXES BY OXIDATION OF FISCHER CARBENE ANIONS AND FERROCENE ENOLATES AND THEIR REACTION

AUTHOR: GEISBAUER A (Reprint); MIHAN S; BECK W

CORPORATE SOURCE: UNIV MUNICH, INST ANORGAN CHEM, D-80333 MUNICH, GERMANY

COUNTRY OF AUTHOR: GERMANY

SOURCE: JOURNAL OF ORGANOMETALLIC CHEMISTRY, (4 OCT 1995)
 Vol. 501, No. 1-2, pp. 61-66.

ISSN: 0022-328X.

PUBLISHER: ELSEVIER SCIENCE SA LAUSANNE, PO BOX 564, 1001 LAUSANNE 1, SWITZERLAND.

DOCUMENT TYPE: Article; Journal

FILE SEGMENT: PHYS

LANGUAGE: German

REFERENCE COUNT: 41

ENTRY DATE: Entered STN: 1995

Last Updated on STN: 1995

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

ED Entered STN: 1995

Last Updated on STN: 1995

AB Oxidative coupling of [(OC)(5)Cr=C(OCH₃)CH₂Li--(+)

and $[\text{FcCOCH}(2)]\text{K}^{--}(+)$ with AgBF_4 gives the dinuclear neutral complexes $(\text{OC})(5)\text{Cr}=\text{C}(\text{OMe})\text{CH}_2\text{CH}_2\text{C}(\text{OMe})=\text{Cr}(\text{CO})(5)$ (1) and $\text{FcCOCH}(2)\text{CH}(2)\text{COFc}$ (2) (Fc = ferrocenyl) in good yield. 1 was characterized by X-ray diffraction. Double **deprotonation** of 1 and 2 with $\text{Bu}(\text{II})\text{Li}$ or KH , respectively, affords dianionic species 3 and 4 which are oxidized to the deeply colored conjugated complexes $(\text{OC})(5)\text{Cr}=\text{C}(\text{OCH}_3)\text{CH}=\text{CHC}(\text{OCH}_3)=\text{Cr}(\text{CO})(3)$ (5) and $\text{FcCOCH}=\text{CHCOFc}$ (6). Addition of the dianion $[(\text{OC})(5)\text{Cr}=\text{C}(\text{OCH}_3)\text{CHCHC}(\text{OCH}_3)=\text{Cr}(\text{CO})(5)](2-)(\text{Li}^+)(2)$ to the cationic **electrophiles** $[\text{Fe}(\text{CO})(3)(\eta(5)-\text{C}_6\text{H}_7)]^+(\text{BF}_4)^-$ and $[\text{Re}(\text{CO})(5)(\eta(2)-\text{C}_2\text{H}_4)]^+(\text{BF}_4)^-$ forms tetranuclear complexes (7, 8) as diastereoisomers. $[\text{FcCOCHCHCOFc}](2-)(\text{K}^+)(2)$ reacts with $[\text{Re}(\text{CO})(5)(\eta(2)-\text{C}_2\text{H}_4)]^+(\text{BF}_4)^-$ to give the trinuclear complex $\text{FcCOCH}(2)\text{CH}[\text{CH}_2\text{CH}_2\text{Re}(\text{CO})(5)]\text{COFc}$ (9).

CC CHEMISTRY, INORGANIC & NUCLEAR; CHEMISTRY, ORGANIC

ST Author Keywords: CHROMIUM; RHENIUM; BRIDGING HYDROCARBON LIGANDS; CRYSTAL STRUCTURE

STP KeyWords Plus (R): TRANSITION-METAL COMPLEXES; CARBON

ABSTRACT IS AVAILABLE IN THE ALL AND IALL FORMATS

L146 ANSWER 113 OF 115 DISSABS COPYRIGHT (C) 2006 ProQuest Information and Learning Company; All Rights Reserved on STN

ACCESSION NUMBER: 1998:10643 DISSABS Order Number: AAR9810694

TITLE: STUDIES ON THE ENANTIOSELECTIVE **DEPROTONATION** OF PHOSPHINE DERIVATIVES WITH ALKYL LITHIUM-(-)-SPARTEINE COMPLEXES

AUTHOR: MUCI, ALEXANDER RAMON [PH.D.]

CORPORATE SOURCE: HARVARD UNIVERSITY (0084)

SOURCE: Dissertation Abstracts International, (1997) Vol. 58, No. 9B, p. 4810. Order No.: AAR9810694. 159 pages.

DOCUMENT TYPE: Dissertation

FILE SEGMENT: DAI

LANGUAGE: English

AB I. Asymmetric Synthesis of P-Chiral Diphosphines via Enantioselective **Deprotonation** with Alkyl lithium-(\$-\$)-Sparteine Complexes. A method for the synthesis of enantiomerically pure P-chiral diphosphines utilizing an enantioselective **deprotonation**-oxidative **coupling** strategy is described. Dimethyl arylphosphine sulfides 15 (X = S) were **deprotonated** with moderate to high enantioselectivities using the n-BuLi-(\$-\$)-sparteine complex (eq 1). Metalation of the analogous phosphine-boranes 16 (X = BH\$\$_3\$) by s-BuLi-(\$-\$)-sparteine proceeded with higher enantioselectivities. Oxidative coupling of the resulting anions with Cu(II) afforded the (S,S)-bis(phosphine-boranes) 25 along with minor amounts of the meso products 26 in moderate to good yield (eq 2). The resulting C\$\$_2\$-symmetric (S,S)-bis(phosphine boranes) 25 were obtained in high enantiomeric purity (>99% ee) after crystallization. Removal of the borane protecting group was effected by treatment with diethylamine to afford the derived diphosphines in high yield.*

II. Enantioselective **Deprotonation** of Cyclic Phosphine Derivatives with Alkyl lithium-(\$-\$)-Sparteine Complexes. Methodology is described where phosphorus-containing heterocycles are enantioselectively metalated with alkyl lithium-(\$-\$)-sparteine complexes. Although phospholane sulfide 10b underwent **deprotonation** in modest enantioselectivity (41-56% ee, eq 3), the analogous phosphorinane derivative 12b was metalated in 99% ee with n-BuLi. Several **electrophiles** were shown to efficiently trap the lithiated phosphacycle. Absolute and relative stereochemistry of 14b was determined by X-ray crystallography of a derived bis(phosphine)rhodium(I) complex. Only one of the two possible diastereomers was observed; the stereochemical outcome is consistent with approach of the

electrophile over the sterically subordinate sulfur.*

III. Kinetic Resolution of Racemic Phosphine Derivatives via Asymmetric Deprotonation with Alkylolithium-(\$-\$)-Sparteine Complexes. The kinetic resolution of racemic phosphine-boranes and sulfides using alkylolithium-(\$-\$)-sparteine complexes was attempted. Several phosphine derivatives were prepared and subjected to reaction with 0.50 equiv of the chiral base (eq 4). Unfortunately, low relative rates of reaction of the two enantiomers (S values) were observed.* ftn*Please refer to the dissertation for diagrams.

CC 0490 CHEMISTRY, ORGANIC

L146 ANSWER 114 OF 115 DISSABS COPYRIGHT (C) 2006 ProQuest Information and Learning Company; All Rights Reserved on STN

ACCESSION NUMBER: 97:8291 DISSABS Order Number: AAR9702683

TITLE: ENANTIOSELECTIVE, LATERAL LITHIATION-SUBSTITUTION REACTIONS USING BENZAMIDE DIRECTING GROUPS

AUTHOR: THAYUMANAVAN, SANKARAN [PH.D.]; BEAK, PETER [advisor]

CORPORATE SOURCE: UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN (0090)

SOURCE: Dissertation Abstracts International, (1996) Vol. 57, No. 8B, p. 5064. Order No.: AAR9702683. 151 pages.

DOCUMENT TYPE: Dissertation

FILE SEGMENT: DAI

LANGUAGE: English

ENTRY DATE: Entered STN: 19970102

Last Updated on STN: 19970102

ED Entered STN: 19970102

Last Updated on STN: 19970102

AB Reactions involving **organolithium** reagents under the influence of the chiral ligand to affect the enantioselective replacement of a carbon-proton bond with a carbon-carbon bond or a carbon-heteroatom bond are described.

Highly enantioenriched substitution products are obtained when N,N-diisopropyl-o-ethylbenzamide is treated with sec-butyllithium/(\$-\$)-sparteine followed by the reaction with **electrophiles**. When the **electrophilic** substitution is carried out with alkyl chlorides as **electrophiles**, the products are obtained with 68-92% ee in moderate to high yields. When alkyl tosylate is used as the **electrophile**, opposite enantiomer of the products are obtained with 78-97% ee in low to high yields.

The enantioselectivity of the reaction can be achieved in one of the three steps in the reaction: the **deprotonation** step, the complexation step, or the substitution step. Tin-lithium exchange experiments of enantioenriched stannyl substrate in the presence and absence of (\$-\$)-sparteine suggests that the enantioselectivity is achieved in the substitution step. **Deprotonation** of racemic N,N-diisopropyl-o-(1\$sp\$prime\$-deutereo)ethylbenzamide using sec-butyllithium/(\$-\$)-sparteine suggests that the initial **deprotonation** reaction proceeds enantioselectively to afford enantioenriched organolithium intermediate which racemizes under the reaction conditions and the enantioselectivity of the product is determined in the substitution step.

Investigation of the enantioselectivity of the products with **electrophiles** with a variety of leaving groups suggested that **electrophiles** with fast and/or non-coordinating electrophiles react with (R)-N,N-(diisopropyl-o-(1\$sp\$prime\$-lithio)ethylbenzamide with inversion of configuration to afford enantioenriched products. Slow and coordinating **electrophiles** react with (R)-N,N-diisopropyl-o-(1\$sp\$prime\$-lithio)ethylbenzamide with retention of configuration to afford products with the opposite enantiomer enriched.

Effect of reaction conditions such as solvent, temperature, directing

groups, substrate structure, and structure of the chiral ligands are also studied.

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ACCESSION NUMBER: 80:29376 DISSABS Order Number: AAR0534605 (not available for sale by UMI)

TITLE: METALATED ALPHA,BETA -UNSATURATED AMIDES IN ORGANIC SYNTHESIS. APPLICATION TO THE SYNTHESIS OF 1-ARYLTETRALIN LIGNANS

AUTHOR: MPANGO, GEORGE BERNARD WILL [PH.D.]

CORPORATE SOURCE: UNIVERSITY OF WATERLOO (CANADA) (1141)

SOURCE: Dissertation Abstracts International, (1980) Vol. 41, No. 12B, p. 4525. Order No.: AAR0534605 (not available for sale by UMI).

DOCUMENT TYPE: Dissertation

FILE SEGMENT: DAI

LANGUAGE: English

ENTRY DATE: Entered STN: 19921118

Last Updated on STN: 19921118

ED Entered STN: 19921118

Last Updated on STN: 19921118

AB The reactions of carbanion derived unsaturated systems with **electrophiles** are reviewed. The Michael reactions of unsaturated systems including tandem conjugate addition-(alpha)-alkylation are summarized and its use in organic synthesis is exemplified.

Part I. The investigation of **lithiated** (alpha),(beta)-unsaturated amides as potential nucleophiles in condensation reactions is described as a general method for **carbon-carbon**

bond formation. **N,N**-

Dimethylcyclohexylideneacetamide and **N,N**-dimethylseneciamide undergo (gamma)-**deprotonation** with **lithium** diisopropylamide

(LDA) to give the **lithiated** species (145, p 112). These species are shown to undergo alkylation, and condensation with aldehydes and ketones, respectively, to give (alpha)-alkylated, (beta),(gamma)-unsaturated amides and (delta)-hydroxyalkylated-(alpha),(beta)-unsaturated amides respectively in good to excellent yields. The regioselectivity of these reactions and the stereochemistry of the products is discussed.

Some (alpha)-alkylated-(beta),(gamma)-unsaturated tertiary amides may be further (alpha)-alkylated giving rise to (alpha),(alpha)-dialkylated-(beta),(gamma)-unsaturated amides in good yield. It was shown that **N**-methyl-(alpha)-(1-methylethenyl)-benzenepropanamide (169, p. 134) could be trilithiated and alkylated at the benzylic position with high selectivity.

Part II. Development of the general methodology of tandem conjugate addition-(alpha)-alkylation of crotonoylpiperidine, **N**-methylcrotonamide and **N,N**-dimethylcrotonamide is described. It is demonstrated that these amides undergo exclusive, 1,4-addition reactions. The resulting enolates may be trapped by **electrophiles** such as methyl iodide, D(,2)O, allylic bromides, and aromatic aldehydes to give (alpha)-alkylated or (beta)-hydroxyalkylated saturated amides.

This methodology was applied to the synthesis of Galcatin and iso-Galcatin as follows: The conjugate addition of aryl dithiane anions to **N,N**-dimethylcrotonamide followed by addition of the appropriate aromatic aldehyde gave a diastereomeric mixture of alcohols in the ratio of 9:1 as determined by NMR and characterization. Treatment of the major isomer with trifluoroacetic acid gave tetralin amide which was successively treated to give Galcatin and iso-Galcatin respectively.

CC 0490 CHEMISTRY, ORGANIC

=> d que 140

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L5      QUE ABB=ON PLU=ON MEUDT, A?/AU
L6      QUE ABB=ON PLU=ON LEHNEMANN, B?/AU
L7      QUE ABB=ON PLU=ON ERBES, M?/AU
L8      QUE ABB=ON PLU=ON FORSTINGER, K?/AU
L9      QUE ABB=ON PLU=ON CLARIANT/PA,CS,SO
L12     QUE ABB=ON PLU=ON DEPROTON? OR (DE(W) PROTON?)
L13     QUE ABB=ON PLU=ON ELECTROPHIL? OR (ELECTRO(W) PHIL?)
L15     QUE ABB=ON PLU=ON "COUPLING REACTION"+PFT,OLD,NT/CT
L18     QUE ABB=ON PLU=ON LITHIATION+PFT,OLD,NT/CT
L19     QUE ABB=ON PLU=ON (CARBON(4A) (N OR O OR S OR P OR NITR
      OGEN OR OXYGEN OR SULFUR OR SULPHUR OR PHOSPHORUS OR HETE
      ROATOM OR (HETERO(W) ATOM)) (7A) (BOND? OR ATTACH? OR LINK
      ?)
L32     1998 SEA FILE=HCAPLUS ABB=ON PLU=ON (L5 OR L6 OR L7 OR L8 OR L9)
L33     20 SEA FILE=HCAPLUS ABB=ON PLU=ON L32 AND (L15 OR L18)
L34     1 SEA FILE=HCAPLUS ABB=ON PLU=ON L33 AND L19
L35     1 SEA FILE=HCAPLUS ABB=ON PLU=ON L33 AND L12
L36     4 SEA FILE=HCAPLUS ABB=ON PLU=ON L33 AND L13
L37     4 SEA FILE=HCAPLUS ABB=ON PLU=ON (L34 OR L35 OR L36)
L38     QUE ABB=ON PLU=ON ORGANOLITH? OR (ORGANO(W) LITH?) OR (
      ORGANIC(W) LITH?)
L39     2 SEA FILE=HCAPLUS ABB=ON PLU=ON L33 AND L38
L40     4 SEA FILE=HCAPLUS ABB=ON PLU=ON L37 OR L39

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=> d que 1131

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L5      QUE ABB=ON PLU=ON MEUDT, A?/AU
L6      QUE ABB=ON PLU=ON LEHNEMANN, B?/AU
L7      QUE ABB=ON PLU=ON ERBES, M?/AU
L8      QUE ABB=ON PLU=ON FORSTINGER, K?/AU
L94     QUE ABB=ON PLU=ON C07F001-02/IPC
L96     QUE ABB=ON PLU=ON (C07B041 OR C07B043 OR C07B045)/IPC
L97     QUE ABB=ON PLU=ON ((N261 OR N262 OR N263) (P) (N341 OR N
      342 OR N343 OR N331 OR N332 OR N333 OR N334 OR N335 OR N3
      52)) /M0,M1,M2,M3,M4,M5,M6
L125     6 SEA FILE=WPIX ABB=ON PLU=ON (L5 OR L6 OR L7 OR L8) AND L94
L126     13 SEA FILE=WPIX ABB=ON PLU=ON (L5 OR L6 OR L7 OR L8) AND L97
L127     8 SEA FILE=WPIX ABB=ON PLU=ON (L5 OR L6 OR L7 OR L8) AND L96
L128     2 SEA FILE=WPIX ABB=ON PLU=ON L125 AND (L126 OR L127)
L130     7 SEA FILE=WPIX ABB=ON PLU=ON L126 AND L127
L131     7 SEA FILE=WPIX ABB=ON PLU=ON L128 OR L130

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=> d his 1141

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      (FILE 'MEDLINE, BIOSIS, EMBASE, PASCAL, JICST-EPLUS, JAPIO, CABA,
      LIFESCI, BIOENG, BIOTECHNO, BIOTECHDS, DRUGU, DRUGB, VETU, VETB,
      SCISEARCH, CONFSCI, DISSABS' ENTERED AT 11:06:11 ON 23 AUG 2006)
L141     1 S L139-L140 AND (L12 OR L13 OR L19)

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=> d que 1141

```

L5      QUE ABB=ON PLU=ON MEUDT, A?/AU
L6      QUE ABB=ON PLU=ON LEHNEMANN, B?/AU
L7      QUE ABB=ON PLU=ON ERBES, M?/AU
L8      QUE ABB=ON PLU=ON FORSTINGER, K?/AU
L9      QUE ABB=ON PLU=ON CLARIANT/PA,CS,SO
L12     QUE ABB=ON PLU=ON DEPROTON? OR (DE(W) PROTON?)
L13     QUE ABB=ON PLU=ON ELECTROPHIL? OR (ELECTRO(W) PHIL?)
L16     QUE ABB=ON PLU=ON LITHIAT? OR LITHIUMIZ? OR LITHIZE?

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L17 QUE ABB=ON PLU=ON LITHIUM OR LI
L19 QUE ABB=ON PLU=ON (CARBON(4A) (N OR O OR S OR P OR NITR
OGEN OR OXYGEN OR SULFUR OR SULPHUR OR PHOSPHORUS OR HETE
ROATOM OR (HETERO(W)ATOM)) (7A) (BOND? OR ATTACH? OR LINK
?)
L38 QUE ABB=ON PLU=ON ORGANOLITH? OR (ORGANO(W)LITH?) OR (
ORGANIC(W)LITH?)
L41 QUE ABB=ON PLU=ON ARYLLITH? OR ALKYLLITH? OR METHYLLIT
H? OR ETHYLLITH? OR PROPYLLITH? OR BUTYLLITH? OR ((ARYL O
R ALKYL OR METHYL OR ETHYL OR PROPYL OR BUTYL) (W) (LI OR L
ITH?))
L138 1521 SEA (L5 OR L6 OR L7 OR L8 OR L9)
L139 1 SEA L138 AND (L16 OR L38 OR L41)
L140 19 SEA L138 AND L17
L141 1 SEA (L139 OR L140) AND (L12 OR L13 OR L19)

=> dup rem l40 l131 l141

FILE 'HCAPLUS' ENTERED AT 11:33:36 ON 23 AUG 2006
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PROCESSING COMPLETED FOR L40
PROCESSING COMPLETED FOR L131
PROCESSING COMPLETED FOR L141
L147 10 DUP REM L40 L131 L141 (2 DUPLICATES REMOVED)
ANSWERS '1-4' FROM FILE HCAPLUS
ANSWERS '5-9' FROM FILE WPIX
ANSWER '10' FROM FILE JAPIO

=> file stnguide

FILE 'STNGUIDE' ENTERED AT 11:33:45 ON 23 AUG 2006
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Aug 18, 2006 (20060818/UP).

=> d ibib ed ab 1-10

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, WPIX, JAPIO' - CONTINUE? (Y)/N:y

L147 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2004:198231 HCAPLUS
DOCUMENT NUMBER: 140:253710
TITLE: preparation of aryllithium compounds using lithium
metal and their reaction with electrophiles.
INVENTOR(S): Meudt, Andreas; Lehnemann, Bernd;
Erbes, Michael; Forstinger, Klaus
PATENT ASSIGNEE(S): Clariant G.m.b.H., Germany
SOURCE: Ger. Offen., 10 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10240262	A1	20040311	DE 2002-10240262	20020831
WO 2004024738	A1	20040325	WO 2003-EP9252	20030821
W: BR, CA, CN, IN, JP, KR, NO, RU, SG, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
EP 1537126	A1	20050608	EP 2003-794907	20030821
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2006131762	A1	20060622	US 2005-526237	20050228
PRIORITY APPLN. INFO.:			DE 2002-10240262	A 20020831
			WO 2003-EP9252	W 20030821

OTHER SOURCE(S): CASREACT 140:253710; MARPAT 140:253710

ED Entered STN: 11 Mar 2004

AB Aryllithium compds. [I, II; Q = Li; R1-R4 = H, Me, (substituted) alkyl, alkoxy, alkylamino, (substituted) Ph, etc.; X1-X4 = C, N; adjoining pairs of X1-X4 = O, S, NH, etc.; Z = CF3, OCF3, Cl, F, alkoxy, aryloxy, alkylthio, arylthio, CH2OH, etc.], were prepared by reaction of Ar-Hal [Ar = (substituted) Ph, naphthyl, biphenyl; Hal = F, Cl, Br, iodo] with Li to give Ar-Li and reaction of Ar-Li with I, II; (Q = H; other variables as above). The resulting aryllithium compds. were reacted with **electrophiles** to give I, II (Q = **electrophile** residue; other variables as above). Thus, 4-ClC6H4Me and furfural di-Et acetal were added to a mixture of Li metal and cat. biphenyl in THF at -65° over 1.5 h; after 9 h tri-Me borate was added over 30 min. followed by stirring for another 30 min. and addition of aqueous HCl to give 81.5% 5-formylfuran-2-boronic acid.

L147 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2004:198229 HCAPLUS

DOCUMENT NUMBER: 140:253119

TITLE: Preparation of organic compounds containing **carbon-heteroatom bonds** using **organolithium** reagents prepared in situ.

INVENTOR(S): Meudt, Andreas; Lehnemann, Bernd; Erbes, Michael; Forstinger, Klaus

PATENT ASSIGNEE(S): Clariant G.m.b.H., Germany

SOURCE: Ger. Offen., 9 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10240260	A1	20040311	DE 2002-10240260	20020831
WO 2004024737	A1	20040325	WO 2003-EP9250	20030821
W: BR, CA, CN, IN, JP, KR, NO, RU, SG, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
EP 1537125	A1	20050608	EP 2003-794905	20030821
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
 JP 2005537331 T2 20051208 JP 2004-535121 20030821
 US 2005258553 A1 20051124 US 2005-526327 20050228
 PRIORITY APPLN. INFO.: DE 2002-10240260 A 20020831
 WO 2003-EP9250 W 20030821

OTHER SOURCE(S): CASREACT 140:253119; MARPAT 140:253119

ED Entered STN: 11 Mar 2004

AB A process for formation of **carbon-heteroatom bonds** comprises (1) treatment of R-Hal (R = Me, (substituted) alkyl, cycloalkyl, Ph, aryl, heteroaryl; Hal = F, Cl, Br, iodo) with Li metal to give RLi, (2) use of RLi for **deprotonation** of R1X1H or R1R2X2H [X1 = O, S, sp²-hybridized N; X2 = sp³-hybridized N; R1, R2 = H, Me, (substituted) alkyl, alkenyl, alkynyl, acyl, alkoxy, aryloxy, dialkylamino, arylamino, heteroaryl, carboxylate, etc.; R1R2 = atoms to form a ring], and (3) treatment of R1X1Li or R1R2X2Li with a carbon **electrophile**. Thus, Li in THF at -35° was treated with 4-ClC6H4Me followed by stirring for ca. 8 h; 2-furylmethanol was added followed by warming to room temperature, addition of propargyl bromide, and reflux for 2 h to give 93% 2-furylmethyl propargyl ether.

L147 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:198230 HCAPLUS

DOCUMENT NUMBER: 140:253342

TITLE: Preparation of derivatized aromatics using organolithium reagents prepared in situ.

INVENTOR(S): Meudt, Andreas; Lehnemann, Bernd; Erbes, Michael; Forstinger, Klaus

PATENT ASSIGNEE(S): Clariant G.m.b.H., Germany

SOURCE: Ger. Offen., 9 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10240261	A1	20040311	DE 2002-10240261	20020831
WO 2004024663	A1	20040325	WO 2003-EP9251	20030821
W: BR, CA, CN, IN, JP, KR, NO, RU, SG, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				

PRIORITY APPLN. INFO.: DE 2002-10240261 A 20020831

OTHER SOURCE(S): CASREACT 140:253342; MARPAT 140:253342

ED Entered STN: 11 Mar 2004

AB Title compds. [I; R1-R5 = H, M, (cyclic) (substituted) alkyl, alkoxy, alkylamino, arylamino, Ph, heteroaryl, alkylthio, arylthio, diarylphosphino, etc.; 2 neighboring R1-R5 = atoms to form a condensed ring; X1-X5 = C, N; Q = **electrophile** residue], were prepared by treatment of Ar-Hal [Ar = (substituted) Ph, pyridyl, naphthyl; Hal = F, Cl, Br, iodo] with Li to give Ar-Li in situ, reaction of the latter with I (Q = Hal; other variables as above) to give I (Q = Li; other variables as above), and treatment of the latter with an **electrophile**. Thus, Li in THF at -35° was treated with 4-ClC6H4Me and cat. biphenyl followed by stirring for 5 h; the mixture was cooled to -70° and treated with 4-BrC6H4CF3. After stirring for 2 h at -50°, Ac2O in THF was added at -30° followed by stirring for 30 min. to give 87.2% 4-trifluoromethylacetophenone.

L147 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:4850 HCAPLUS
DOCUMENT NUMBER: 138:73075
TITLE: Process for the preparation of substituted aromatics
via lithiation and electrophilic alkylation
of haloaromatics
INVENTOR(S): Meudt, Andreas; Erbes, Michael;
Forstinger, Klaus
PATENT ASSIGNEE(S): Clariant G.m.b.H., Germany
SOURCE: Eur. Pat. Appl., 11 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1270535	A2	20030102	EP 2002-12763	20020608
EP 1270535	A3	20040218		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
DE 10155209	A1	20030109	DE 2001-10155209	20011109
US 2003018192	A1	20030123	US 2002-171444	20020613
US 6657093	B2	20031202		
JP 2003073308	A2	20030312	JP 2002-180218	20020620
US 2004073032	A1	20040415	US 2003-677412	20031002
US 7022857	B2	20060404		
PRIORITY APPLN. INFO.:			DE 2001-10129765	A 20010620
			DE 2001-10155209	A 20011109
			US 2002-171444	A3 20020613
OTHER SOURCE(S):		CASREACT 138:73075; MARPAT 138:73075		
ED	Entered STN: 03 Jan 2003			
AB	A process for the preparation of compds. I [R1 - R5 = H, (un)substituted alkyl, alkoxy, etc.; R6 = aryl, alkyl] via the lithiation and electrophilic alkylation of haloaroms. I [R1 - R5 = H, (un)substituted alkyl, alkoxy, etc.; R6 = Cl, F] is disclosed. For example, a mixture of p-chlorotoluene (1 mol) and acetonitrile (1.1 mol) was added to a suspension of lithium (2.0 mol) in THF (350 mL) at -50°C. After stirring for 7.5 h, the reaction was quenched with water, the pH adjusted to 2.0 and the mixture heated at reflux for 2 h. The reaction was cooled, extracted with petroleum ether and the combined organic layers were distilled to provide acetophenone II in 99% yield. The preparation of approx. 12-specific examples of compds. I are disclosed.			

L147 ANSWER 5 OF 10 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
ACCESSION NUMBER: 2005-786034 [80] WPIX
DOC. NO. CPI: C2005-241887
TITLE: Preparation of aldehydes, useful as intermediates in organic synthesis, comprises reaction of primary and secondary alcohols with cyclic phosphonic acid anhydrides in the presence of dialkyl-, diaryl- and/or alkyl-aryl sulfonic oxides.
DERWENT CLASS: E19
INVENTOR(S): BOEHM, C; MEUDT, A; SCHERER, S
PATENT ASSIGNEE(S): (CLRN) CLARIANT GMBH
COUNTRY COUNT: 110
PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
WO 2005102978	A1	20051103	(200580)*	GE	16
RW: AT BE BG BW CH CY CZ DE DK EA EE ES FI FR GB GH GM GR HU IE IS IT KE LS LT LU MC MW MZ NA NL OA PL PT RO SD SE SI SK SL SZ TR TZ UG ZM ZW					
W: AE AG AL AM AT AU AZ BA BB BG BR BW BY BZ CA CH CN CO CR CU CZ DK DM DZ EC EE EG ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KM KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NA NI NO NZ OM PG PH PL PT RO RU SC SD SE SG SK SL SM SY TJ TM TN TR TT TZ UA UG US UZ VC VN YU ZA ZM ZW					
DE 102004020189	A1	20051117	(200580)		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2005102978	A1	WO 2005-EP4093	20050418
DE 102004020189	A1	DE 2004-102004020189	20040422

PRIORITY APPLN. INFO: DE 2004-102004020189 20040422

ED 20051213

AB WO2005102978 A UPAB: 20051213

NOVELTY - Preparation of aldehydes comprises reaction of primary alcohols or secondary alcohols with cyclic phosphonic acid anhydrides in the presence of dialkyl-, diaryl- and/or alkyl-aryl sulfonic oxides at -100 to +120 deg. C.

DETAILED DESCRIPTION - Preparation of aldehydes of formula ((R1-CHO) or R1-C(O)-R2)) comprises reaction of primary alcohols of formula (R1CH2-OH) or secondary alcohols of formula (R1-CH(OH)-R2) with cyclic phosphonic acid anhydrides in the presence of dialkyl-, diaryl- and/or alkyl-aryl sulfonic oxides at -100 to +120 deg. C.

R1, R2 = substituted 1-12C alkyl, substituted 3-10C cycloalkyl-, alkenyl- or (hetero)aryl.

USE - The aldehydes are useful as intermediates in various organic synthesis.

ADVANTAGE - The oxidation of primary and secondary alcohols to appropriate aldehydes and/or ketones takes place at very mild reaction conditions and in a simplified process. The process is economical and the formed intermediate exhibits high stability.

Dwg.0/0

L147 ANSWER 6 OF 10 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN

ACCESSION NUMBER: 2005-555480 [56] WPIX

DOC. NO. CPI: C2005-167355

TITLE: Preparation of nitriles and isonitriles, useful as intermediates in organic synthesis by heterocarbonyl reaction, involves dehydration of carboxamide, ammonium carboxylate, formamide or precursors with cyclic phosphonic anhydride.

DERWENT CLASS: E11 E19

INVENTOR(S): MEUDT, A; NERDINGER, S; SCHERER, S

PATENT ASSIGNEE(S): (CLRN) CLARIANT GMBH

COUNTRY COUNT: 108

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
WO 2005070879	A1	20050804	(200556)*	GE	16

RW: AT BE BG BW CH CY CZ DE DK EA EE ES FI FR GB GH GM GR HU IE IS IT
KE LS LT LU MC MW MZ NA NL OA PL PT RO SD SE SI SK SL SZ TR TZ UG
ZM ZW

W: AE AG AL AM AT AU AZ BA BB BG BR BW BY BZ CA CH CN CO CR CU CZ DK
DM DZ EC EE EG ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP
KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NA NI NO NZ OM
PG PH PL PT RO RU SC SD SE SG SK SL SY TJ TM TN TR TT TZ UA UG US
UZ VC VN YU ZA ZM ZW

DE 102004003953 A1 20050811 (200556)

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2005070879	A1	WO 2005-EP361	20050115
DE 102004003953	A1	DE 2004-102004003953	20040126

PRIORITY APPLN. INFO: DE 2004-102004003953 20040126

ED 20050902

AB WO2005070879 A UPAB: 20050902

NOVELTY - Preparation of nitriles (II) and isonitriles (III) with a (cyclo)alkyl, alkenyl, alkynyl or (hetero)aryl group comprises reacting (a) carboxamides, ammonium carboxylates or carboxylic acids in the presence of ammonia or ammonium salts or (b) formamides or mixtures of amines and formic acid with cyclic phosphonic anhydrides at -30 to +120 deg. C, with elimination of water.

DETAILED DESCRIPTION - Preparation of nitriles R-CN (II) and isonitriles R-NC (III) with a (cyclo)alkyl, alkenyl, alkynyl or (hetero)aryl group comprises reacting (a) carboxamides (RCO-NH₂), ammonium carboxylates (RCOO-NH₄⁺) or carboxylic acids in the presence of ammonia or ammonium salts (RCOOH + NH₃, RCOOH + NH₄⁺) or (b) formamides H-CO-NHR or mixtures of amines and formic acid with cyclic phosphonic anhydrides (I) at -30 to +120 deg. C, with elimination of water, where:

R = any substituted linear or branched 1-8 C alkyl, 3-10 C cycloalkyl, alkenyl, alkynyl, aryl or heteroaryl group:

USE - Nitriles (II) and isonitriles (III) are widely useful as intermediates in organic synthesis and can be used in an infinite number of heterocarbonyl reactions.

ADVANTAGE - The process allows dehydration of carboxylic acids, ammonium carboxylates and amides to the corresponding nitriles and of formamides to the corresponding isonitriles, has very high chemoselectivity and is economically useful. It avoids epimerization and gives maximum regio- and stereoselectivity. The yields are typically 90-100%, especially over 95% and selectivity 97-100, especially 99-100%.
Dwg.0/0

L147 ANSWER 7 OF 10 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN

ACCESSION NUMBER: 2004-582009 [57] WPIX

DOC. NO. CPI: C2004-212494

TITLE: Production of beta-keto carboxylic acid derivatives, e.g. useful as pharmaceutical, agrochemical or dye intermediates, comprises continuously reacting diketenes with active hydrogen compounds in a microreactor.

DERWENT CLASS: B05 C03 E19

INVENTOR(S): FORSTINGER, K; KIM, H; NICKEL, U; UNVERDORBEN, L; WEHLE, D

PATENT ASSIGNEE(S): (CLRN) CLARIANT GMBH; (FORS-I) FORSTINGER K; (KIMH-I) KIM H; (NICK-I) NICKEL U; (UNVE-I) UNVERDORBEN L; (WEHL-I) WEHLE D

COUNTRY COUNT: 31
PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
DE 10303581	A1	20040812	(200457)*		9
WO 2004067492	A1	20040812	(200457)	GE	
RW: AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IT LU MC NL PT RO					
SE SI SK TR					
W: CN JP KR US					
EP 1590315	A1	20051102	(200573)	GE	
R: AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IT LI LU MC NL PT					
RO SE SI SK TR					
JP 2006514079	W	20060427	(200628)		19
US 2006142588	A1	20060629	(200643)		
KR 2005095908	A	20051004	(200648)		
CN 1745056	A	20060308	(200649)		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
DE 10303581	A1	DE 2003-10303581	20030130
WO 2004067492	A1	WO 2003-EP14200	20031213
EP 1590315	A1	EP 2003-789268	20031213
		WO 2003-EP14200	20031213
JP 2006514079	W	WO 2003-EP14200	20031213
		JP 2004-567309	20031213
US 2006142588	A1	WO 2003-EP14200	20031213
		US 2005-544076	20050729
KR 2005095908	A	WO 2003-EP14200	20031213
		KR 2005-713908	20050728
CN 1745056	A	CN 2003-80109365	20031213

FILING DETAILS:

PATENT NO	KIND	PATENT NO
EP 1590315	A1 Based on	WO 2004067492
JP 2006514079	W Based on	WO 2004067492
KR 2005095908	A Based on	WO 2004067492

PRIORITY APPLN. INFO: DE 2003-10303581 20030130

ED 20040907

AB DE 10303581 A UPAB: 20040907

NOVELTY - Production of beta -keto carboxylic acid derivatives (I) by reacting diketenes (II) with active hydrogen compounds comprises carrying out the reaction continuously in a microreactor.

DETAILED DESCRIPTION - Production of beta -keto carboxylic acid derivatives of formula (I) by reacting diketenes of formula (II) with active hydrogen compounds of formula RXH comprises carrying out the reaction continuously in a microreactor.

X = NR', O or S;

R, R' = H or optionally substituted 1-18C (cyclo)alkyl, (cyclo)alkenyl, aryl or heteroaryl;

R1-R4 = H or optionally substituted 1-18C (cyclo)alkyl, (cyclo)alkenyl, aryl or heteroaryl;

R1+R2, R3+R4 = (CH2)k; and

k = 2-6.

USE - Acetoacetyl esters are useful as intermediates for

pharmaceuticals, dyes and agrochemicals. Acetoacetyl amides are useful as intermediates for pigments and reactive dyes.

ADVANTAGE - The process gives very pure products in good yields and has safety and environmental benefits.

Dwg.0/0

L147 ANSWER 8 OF 10 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
 ACCESSION NUMBER: 2001-267527 [28] WPIX
 DOC. NO. CPI: C2001-081194
 TITLE: Production of aromatic amines, comprises reacting aryl halides with an amine in the presence of a palladium phosphacyclobutane complex, useful as intermediates for dyes, fine chemicals, agrochemicals and pharmaceuticals.
 DERWENT CLASS: B05 C03 E13 E19
 INVENTOR(S): GEISSLER, H; HABER, S; MEUDT, A; SCHERER, S; VOLLMUELLER, F
 PATENT ASSIGNEE(S): (CLRN) CLARIANT GMBH
 COUNTRY COUNT: 27
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
EP 1083163	A2	20010314	(200128)*	GE	9
R: AL AT BE CH CY DE DK ES FI FR GB GR IE IT LI LT LU LV MC MK NL PT RO SE SI					
DE 19942961	A1	20010315	(200128)		
JP 2001151732	A	20010605	(200138)		8
US 6353136	B1	20020305	(200224)		

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
EP 1083163	A2	EP 2000-118912	20000901
DE 19942961	A1	DE 1999-1042961	19990909
JP 2001151732	A	JP 2000-275094	20000911
US 6353136	B1	US 2000-658830	20000908

PRIORITY APPLN. INFO: DE 1999-19942961 19990909

ED 20010522

AB EP 1083163 A UPAB: 20010522

NOVELTY - Production of aromatic amines (I) comprises reacting aryl halides (II) with an amine (III) in the presence of a palladium (Pd) phosphacyclobutane complex (IV) and a base in a solvent at 20-200 deg. C.

DETAILED DESCRIPTION - Production of aromatic amines of formula (I) comprises reacting aryl halides of formula (II) with an amine of formula (III) in the presence of a palladium (Pd) phosphacyclobutane complex of formula (IV) and a base, and optionally an ionic halide, in a solvent at 20-200 deg. C.

n = 1-3;

X = F, Cl or Br;

Ar = phenyl, furyl, pyrrolyl, pyridyl, naphthyl or quinolinyl, all optionally substituted by 1-6 of 1-8C alkyl, 3-8C cycloalkyl, 1-8C alkoxy, 1-8C acyloxy, 6-10C aryloxy, 6-10C aryl, benzyl, F, Cl, Br, OH, NO₂, OSO₂CF₃, CN, COOH, CHO, SO₃H, SO₂R, NH₂, NHA, NAA, NHCOA, N(A)COA, COOA, CONH₂, COA, NHCHO, NHCOOA, CPh, COOPh, CH=CHCOOA, CH=CHCOOH, POPh₂, POA₂ and 5- or 6-membered heteroaryl;

A = 1-8C alkyl;

R = A, 6-10C aryl or benzyl;

R6, R7 = H, 1-12C alkyl, 1-12C hydroxyalkyl, optionally substituted phenyl or 3-8C cycloalkyl; or

NR6R7 = 5- or 6-membered aliphatic or aromatic ring optionally containing 1-2 other heteroatoms selected from N, O and S;

R1a, R2a = H, A', 3-12C cycloalkyl, OA', F, NA'A', COOA', OCOA' or optionally substituted aryl;

A' = 1-4C alkyl; or

R3a, R4a, R5a, R6a = 1-8C alkyl, 3-12C cycloalkyl of optionally substituted aryl;

R1a+R2a or R2a+R3a or R3a+R4a = 4-10C aliphatic ring; or

R5a+R6a = 4- to 9-membered ring; or

R4a+R5a = 2-7C alkylene bridge; and

Y = an (in)organic anion, an alpha, gamma -diketo compound or a 5- or 6-membered N-containing heterocycle.

USE - The process is useful for producing amino-substituted benzene, furan, pyrrole and pyridine derivatives, especially anilines, which are useful as intermediates for dyes, fine chemicals, agrochemicals and pharmaceuticals.

ADVANTAGE - The process gives high yields, e.g. 48-91%.

Dwg.0/0

L147 ANSWER 9 OF 10 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
 ACCESSION NUMBER: 2001-062452 [08] WPIX
 DOC. NO. CPI: C2001-017545
 TITLE: New palladium and nickel complexes of
 2'-hydroxy-biphenyl-2-yl-phosphane compounds useful as
 catalysts for coupling aryl or alkyl metallate, phenol,
 phenolate, alcohol, alkoxide, amine or amide with aryl
 halide or sulfonate.
 DERWENT CLASS: A60 E11 E19
 INVENTOR(S): HABER, S; MEUDT, A; NOERENBERG, A; SCHERER, S;
 VOLLMUELLER, F
 PATENT ASSIGNEE(S): (CLRN) CLARIANT GMBH
 COUNTRY COUNT: 25
 PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG
DE 19920847	A1	20001109	(200108)*		13
WO 2000068237	A1	20001116	(200108)	GE	
RW: AT BE CH CY DE DK ES FI FR GB GR IE IT LU MC NL PT SE					
W: BR CA CN IL JP KR MX					

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
DE 19920847	A1	DE 1999-1020847	19990506
WO 2000068237	A1	WO 2000-EP3710	20000426

PRIORITY APPLN. INFO: DE 1999-19920847 19990506

ED 20010207

AB DE 19920847 A UPAB: 20010207

NOVELTY - Complexes of palladium (Pd) or nickel (Ni) and a
 2'-hydroxy-biphenyl-2-yl-phosphane compound (I) are new.

DETAILED DESCRIPTION - Complexes of palladium (Pd) or nickel (Ni) and
 a 2'-hydroxy-biphenyl-2-yl-phosphane compound of formula (I) are new.

R1, R2 = linear or branched 1-8 carbon (C) alkyl, 4-8 C cycloalkyl,
 2-12 C alkenyl, 2-12 C alkynyl, a phenyl group (with 0-3 substituents)

selected from 1-4 C alkyl, 1-4 C alkoxy, fluorine (F) or trifluoromethyl (CF₃) or heteroaryl; or

R1R2 = a 3-8 C 1, omega -alkendiyl chain;

R3 = hydrogen (H), 1-12 C alkyl, 2-12 C alkenyl, 2-12 C alkynyl, phenyl, naphthyl, heteroaryl, lithium (Li), sodium (Na), potassium (K), chloromagnesium (MgCl), bromomagnesium (MgBr), iodomagnesium (MgI), Mg0.5, chlorozinc (ZnCl), bromozinc (ZnBr), Zn0.5, PO-phenyl₂, PO-(1-8 C alkyl)₂, PO₃-(1-8 C alkyl)₂, SO₂R, SO₂R', SiR₃, C(=O)R, C(=O)NR₂, C(=O)NHR, C(=O)OR; or a polymer matrix linked to the phenolic oxygen (O) atom directly or by an (ar)aliphatic or aromatic bridge;

R = 1-4 C alkyl, CF₃, phenyl or tolyl;

R4-11 = H, 1-12 C alkyl, 2-12 C alkenyl, 2-12 C alkynyl, phenyl, OSO₂R' or SiR'₃; or

one pair of adjacent groups R4-11 = a condensed benzo group with 4 R' substituents; and

R' = H, 1-12 C alkyl or phenyl.

The full definitions are given in the DEFINITIONS (Full Definitions) Field.

An INDEPENDENT CLAIM is also included for the preparation of (I).

USE - The complexes are used as catalysts for C,C-, C,N- and C,O-coupling of aryl metallates, alkyl metallates, phenols, phenolates, alcohols, alkoxides, amines or amides with aryl halides, preferably aryl chlorides, or aryl sulfonates (all claimed) to biaryls, styrenes, phenylacetylenes, anilines, phenol ethers and diaryl ethers that are important intermediates in the chemical industry.

ADVANTAGE - These catalyst systems allow simple and cost-effective C,C-, C,N- and C,O-coupling reaction of chloroaromatics with good yields. They are very effective in Suzuki, Grignard and Stille couplings and couplings of arylsilanes and arylzinc compounds and also show high reaction velocities in Heck reactions of olefins and acetylenes. Even unactivated chloroaromatics can be converted to the desired products with high yields.

Dwg.0/0

L147 ANSWER 10 OF 10 JAPIO (C) 2006 JPO on STN

ACCESSION NUMBER: 2003-073308 JAPIO
 TITLE: METHOD FOR PRODUCING SUBSTITUTED AROMATIC COMPOUND
 INVENTOR: MEUDT ANDREAS DR; ERBES MICHAEL;
 FORSTINGER KLAUS
 PATENT ASSIGNEE(S): CLARIANT GMBH
 PATENT INFORMATION:

PATENT NO	KIND	DATE	ERA	MAIN IPC
JP 2003073308	A	20030312	Heisei	C07C002-68

APPLICATION INFORMATION

STN FORMAT: JP 2002-180218 20020620
 ORIGINAL: JP2002180218 Heisei
 PRIORITY APPLN. INFO.: DE 2001-10129765 20010620
 PRIORITY APPLN. INFO.: DE 2001-10155209 20011109
 SOURCE: PATENT ABSTRACTS OF JAPAN (CD-ROM), Unexamined Applications, Vol. 2003

ED 20030709

AB PROBLEM TO BE SOLVED: To provide a method for efficiently producing an aryl- or alkyl- substituted aromatic compound and heteroaromatic compound in a costwise effective way attaining good yield and high purity.
 SOLUTION: This method for producing the aryl- or alkyl-substituted aromatic compound and heteroaromatic compound includes to react a chloroaromatic compound or a fluoroaromatic compound with an

electrophilic carbon material and lithium metal.
COPYRIGHT: (C) 2003, JPO

=> d his ful

(FILE 'HOME' ENTERED AT 08:51:31 ON 23 AUG 2006)

FILE 'ZCAPLUS' ENTERED AT 08:51:49 ON 23 AUG 2006
E US2005-526327/APPS

L1 FILE 'HCAPLUS' ENTERED AT 08:52:54 ON 23 AUG 2006
1 SEA ABB=ON PLU=ON US2005-526327/APPS
SAVE TEMP L1 KUM327HCAAPP/A

FILE 'STNGUIDE' ENTERED AT 08:53:13 ON 23 AUG 2006

FILE 'HCAPLUS' ENTERED AT 08:53:17 ON 23 AUG 2006
D IBIB ED AB IND

FILE 'STNGUIDE' ENTERED AT 08:53:18 ON 23 AUG 2006

L2 FILE 'WPIX' ENTERED AT 08:55:35 ON 23 AUG 2006
1 SEA ABB=ON PLU=ON US2005-526327/APPS
SAVE TEMP L2 KUM327WPIAPP/A
D IALL CODE

FILE 'STNGUIDE' ENTERED AT 08:56:07 ON 23 AUG 2006

FILE 'REGISTRY' ENTERED AT 08:57:39 ON 23 AUG 2006

L3 FILE 'HCAPLUS' ENTERED AT 08:57:43 ON 23 AUG 2006
TRA PLU=ON L1 1- RN : 23 TERMS

L4 FILE 'REGISTRY' ENTERED AT 08:57:47 ON 23 AUG 2006
23 SEA ABB=ON PLU=ON L3
SAVE TEMP L4 KUM327REGAPP/A
D SCAN

FILE 'STNGUIDE' ENTERED AT 08:58:14 ON 23 AUG 2006

L5 FILE 'ZCAPLUS' ENTERED AT 09:00:02 ON 23 AUG 2006
L6 QUE ABB=ON PLU=ON MEUDT, A?/AU
L7 QUE ABB=ON PLU=ON LEHNEMANN, B?/AU
L8 QUE ABB=ON PLU=ON ERBES, M?/AU
L9 QUE ABB=ON PLU=ON FORSTINGER, K?/AU
L10 QUE ABB=ON PLU=ON CLARIANT/PA,CS,SO
L11 QUE ABB=ON PLU=ON AY<2004 OR PY<2004 OR PRY<2004 OR MY<2004
OR REVIEW/DT
L12 QUE ABB=ON PLU=ON AY<2004 OR PY<2004 OR PRY<2004
L13 QUE ABB=ON PLU=ON DEPROTON? OR (DE(W) PROTON?)
L14 QUE ABB=ON PLU=ON ELECTROPHIL? OR (ELECTRO(W) PHIL?)
L14 QUE ABB=ON PLU=ON COUPLING
L*** DEL QUE "COUPLING REACTION"/TI,IT,CC,CT,ST,STP
L15 QUE ABB=ON PLU=ON "COUPLING REACTION"+PFT,OLD,NT/CT
L16 QUE ABB=ON PLU=ON LITHIAT? OR LITHIUMIZ? OR LITHIZE?
L17 QUE ABB=ON PLU=ON LITHIUM OR LI
L18 QUE ABB=ON PLU=ON LITHIATION+PFT,OLD,NT/CT
L19 QUE ABB=ON PLU=ON (CARBON(4A) (N OR O OR S OR P OR NITROGEN
OR OXYGEN OR SULFUR OR SULPHUR OR PHOSPHORUS OR HETEROATOM OR
(HETERO(W)ATOM)) (7A) (BOND? OR ATTACH? OR LINK?)
L20 QUE ABB=ON PLU=ON FORM OR FORMED OR FORMING OR FORMS OR
FORMATION OR GENERAT?

L21 FILE 'LREGISTRY' ENTERED AT 09:08:42 ON 23 AUG 2006
STR

L22 FILE 'REGISTRY' ENTERED AT 09:09:05 ON 23 AUG 2006
50 SEA SSS SAM L21
D QUE STAT

FILE 'STNGUIDE' ENTERED AT 09:10:06 ON 23 AUG 2006

L23 FILE 'LREGISTRY' ENTERED AT 09:13:49 ON 23 AUG 2006
STR L21

L24 FILE 'REGISTRY' ENTERED AT 09:15:44 ON 23 AUG 2006
50 SEA SSS SAM L23
D QUE STAT

L25 5136 SEA SSS FUL L23
SAVE TEMP L25 KUM327LIQ/A

FILE 'STNGUIDE' ENTERED AT 09:18:11 ON 23 AUG 2006

L26 FILE 'REGISTRY' ENTERED AT 09:18:38 ON 23 AUG 2006
152 SEA ABB=ON PLU=ON L25 AND USPATFULL/LC

L27 38 SEA ABB=ON PLU=ON L25 AND USPAT2/LC

L28 81 SEA ABB=ON PLU=ON L25 AND TOXCENTER/LC

L29 1 SEA ABB=ON PLU=ON L25 AND MEDLINE/LC

L30 11 SEA ABB=ON PLU=ON L25 AND BIOSIS/LC

L*** DEL 0 S L25 AND EMBASE/LS

L31 1 SEA ABB=ON PLU=ON L25 AND EMBASE/LC

FILE 'STNGUIDE' ENTERED AT 09:19:58 ON 23 AUG 2006

FILE 'REGISTRY' ENTERED AT 09:20:43 ON 23 AUG 2006

L32 FILE 'HCAPLUS' ENTERED AT 09:20:46 ON 23 AUG 2006
1998 SEA ABB=ON PLU=ON (L5 OR L6 OR L7 OR L8 OR L9)

L33 20 SEA ABB=ON PLU=ON L32 AND (L15 OR L18)

L34 1 SEA ABB=ON PLU=ON L33 AND L19

L35 1 SEA ABB=ON PLU=ON L33 AND L12

L36 4 SEA ABB=ON PLU=ON L33 AND L13

L37 4 SEA ABB=ON PLU=ON (L34 OR L35 OR L36)
D SCAN

FILE 'STNGUIDE' ENTERED AT 09:22:05 ON 23 AUG 2006

L38 FILE 'ZCAPLUS' ENTERED AT 09:22:23 ON 23 AUG 2006
QUE ABB=ON PLU=ON ORGANOLITH? OR (ORGANO(W)LITH?) OR
(ORGANIC(W)LITH?)

L39 FILE 'HCAPLUS' ENTERED AT 09:22:57 ON 23 AUG 2006
2 SEA ABB=ON PLU=ON L33 AND L38

L40 4 SEA ABB=ON PLU=ON L37 OR L39
D SCAN

FILE 'STNGUIDE' ENTERED AT 09:23:24 ON 23 AUG 2006

FILE 'HCAPLUS' ENTERED AT 09:24:41 ON 23 AUG 2006
SAVE TEMP L40 KUM327HCAINV/A

FILE 'STNGUIDE' ENTERED AT 09:24:58 ON 23 AUG 2006

FILE 'ZCAPLUS' ENTERED AT 09:25:08 ON 23 AUG 2006
L41 QUE ABB=ON PLU=ON ARYLLITH? OR ALKYLLITH? OR METHYLLITH? OR
ETHYLLITH? OR PROPYLLITH? OR BUTYLLITH? OR ((ARYL OR ALKYL OR
METHYL OR ETHYL OR PROPYL OR BUTYL) (W) (LI OR LITH?))

FILE 'HCAPLUS' ENTERED AT 09:26:38 ON 23 AUG 2006
L42 0 SEA ABB=ON PLU=ON L1 NOT L40
L43 4767 SEA ABB=ON PLU=ON L25 (L) RACT/RL
L44 138 SEA ABB=ON PLU=ON L25 (L) (L38 OR L41 OR L16 OR L19)
L45 58 SEA ABB=ON PLU=ON L43 AND L44
L46 61 SEA ABB=ON PLU=ON L43 AND (L15 OR L18)
L47 187 SEA ABB=ON PLU=ON (L44 OR L45 OR L46) AND (L12 OR L13 OR L14
OR L16 OR L19 OR L20 OR L38 OR L41)
L48 152 SEA ABB=ON PLU=ON L47 AND L10
L49 37 SEA ABB=ON PLU=ON (L15 OR L18) (L) L19
L50 251 SEA ABB=ON PLU=ON (L15 OR L18) (L) (L38 OR L41)
L51 69 SEA ABB=ON PLU=ON (L49 OR L50) AND (L12 OR L13)
L52 62 SEA ABB=ON PLU=ON L51 AND L10
L53 158 SEA ABB=ON PLU=ON (L48 OR L52) AND ORGAN?/SC,SX
L54 25 SEA ABB=ON PLU=ON L53 AND L12
L55 51 SEA ABB=ON PLU=ON L53 AND L13
L56 7 SEA ABB=ON PLU=ON L54 AND L55
D SCAN TI HIT
L57 155 SEA ABB=ON PLU=ON (L48 OR L52) AND ORGANIC/SC,SX
L58 69 SEA ABB=ON PLU=ON L54 OR L55
L59 0 SEA ABB=ON PLU=ON L1 NOT L58
SAVE TEMP L58 KUM327HCA1B/AQ KUM327HCA1B/A

FILE 'STNGUIDE' ENTERED AT 09:37:01 ON 23 AUG 2006
D SAVED

FILE 'LREGISTRY' ENTERED AT 09:39:04 ON 23 AUG 2006
L60 STR L23

FILE 'REGISTRY' ENTERED AT 09:40:09 ON 23 AUG 2006
L61 50 SEA SSS SAM L60
D QUE STAT
L62 8814 SEA SSS FUL L60
SAVE TEMP L62 KUM327LIQ2/A

FILE 'STNGUIDE' ENTERED AT 09:41:26 ON 23 AUG 2006
D SAVED

FILE 'REGISTRY' ENTERED AT 09:41:51 ON 23 AUG 2006
L63 181 SEA ABB=ON PLU=ON L62 AND USPATFULL/LC
L64 39 SEA ABB=ON PLU=ON L62 AND USPAT2/LC
L65 1 SEA ABB=ON PLU=ON L62 AND MEDLINE/LC
L66 11 SEA ABB=ON PLU=ON L62 AND BIOSIS/LC
L67 1 SEA ABB=ON PLU=ON L62 AND EMBASE/LC

FILE 'HCAPLUS' ENTERED AT 09:43:06 ON 23 AUG 2006
L68 5309 SEA ABB=ON PLU=ON L62 (L) (RACT+NT)/RL
L69 376 SEA ABB=ON PLU=ON L62 (L) (L14 OR L16 OR L19 OR L38 OR L41)
L70 125 SEA ABB=ON PLU=ON L68 AND L69
L71 104 SEA ABB=ON PLU=ON L69 AND (L15 OR L18)
L72 144 SEA ABB=ON PLU=ON (L70 OR L71) AND L10
L73 14 SEA ABB=ON PLU=ON L72 AND (L12 OR L13)
L74 3 SEA ABB=ON PLU=ON L73 AND (L14 OR L19)
D SCAN TI HIT

L75 11 SEA ABB=ON PLU=ON L73 AND ORGANIC/SC,SX
L76 14 SEA ABB=ON PLU=ON (L73 OR L74 OR L75)
L77 2 SEA ABB=ON PLU=ON L76 AND L12 AND L13
D SCAN TI HIT
L78 71 SEA ABB=ON PLU=ON L58 OR L77
SAVE TEMP L78 KUM327HCA2B/A

FILE 'STNGUIDE' ENTERED AT 09:48:03 ON 23 AUG 2006

FILE 'LREGISTRY' ENTERED AT 09:48:51 ON 23 AUG 2006
D QUE STAT L62
L79 STR L60

FILE 'STNGUIDE' ENTERED AT 09:51:21 ON 23 AUG 2006

FILE 'CASREACT' ENTERED AT 09:51:59 ON 23 AUG 2006
L80 27 SEA SSS SAM L79 (916 REACTIONS)
D QUE STAT

FILE 'STNGUIDE' ENTERED AT 09:52:54 ON 23 AUG 2006

FILE 'CASREACT' ENTERED AT 09:56:11 ON 23 AUG 2006
L81 7132 SEA ABB=ON PLU=ON L62/NPRO

FILE 'STNGUIDE' ENTERED AT 09:56:26 ON 23 AUG 2006
D QUE STAT L80

FILE 'CASREACT' ENTERED AT 09:56:52 ON 23 AUG 2006

FILE 'STNGUIDE' ENTERED AT 09:57:29 ON 23 AUG 2006

FILE 'CASREACT' ENTERED AT 09:58:21 ON 23 AUG 2006
L82 7715 SEA ABB=ON PLU=ON L62
L83 1756 SEA ABB=ON PLU=ON L82 AND (L14 OR L16 OR L19 OR L38 OR L41)
L84 1756 SEA ABB=ON PLU=ON L82 AND ((COUPLING/BI,AB) OR (LITHIAT?/BI,AB
OR LITHIUMIZ?/BI,AB OR LITHIZE?/BI,AB) OR ((CARBON/BI,AB(4A) (N/BI,AB OR O/BI,AB OR S/BI,AB OR P/BI,AB OR NITROGEN/BI,AB OR
OXYGEN/BI,AB OR SULFUR/BI,AB OR SULPHUR/BI,AB OR PHOSPHORUS/BI,AB OR HETEROATOM/BI,AB OR (HETERO/BI,AB(W)ATOM/BI,AB))) (7A)
(BOND?/BI,AB OR ATTACH?/BI,AB OR LINK?/BI,AB) OR (ORGANOLITH?/BI,AB OR (ORGANO/BI,AB(W)LITH?/BI,AB) OR (ORGANIC/BI,AB(W)LITH?
/BI,AB) OR (ARYLLITH?/BI,AB OR ALKYLITH?/BI,AB OR METHYLLITH?/BI,AB OR ETHYLLITH?/BI,AB OR PROPYLLITH?/BI,AB OR BUTYLLITH?/BI,AB OR
I,AB OR ((ARYL/BI,AB OR ALKYL/BI,AB OR METHYL/BI,AB OR ETHYL/BI,AB OR PROPYL/BI,AB OR BUTYL/BI,AB) (W) (LI/BI,AB OR
LITH?/BI,AB))))
L85 94 SEA ABB=ON PLU=ON L84 AND (DEPROTON?/BI,AB OR (DE/BI,AB(W)PRO
TON?/BI,AB))
L86 51 SEA ABB=ON PLU=ON L84 AND (ELECTROPHIL?/BI,AB OR (ELECTRO/BI,
AB(W)PHIL?/BI,AB))
L87 5 SEA ABB=ON PLU=ON L85 AND L86
L88 110 SEA ABB=ON PLU=ON (L85 OR L86) AND L10
L89 98 SEA ABB=ON PLU=ON L88 AND ORGANIC/SC,SX
L90 4 SEA ABB=ON PLU=ON L87 AND L88
L*** DEL 98 S L88 AND L89
L91 4 SEA ABB=ON PLU=ON L87 AND L89
L92 4 SEA ABB=ON PLU=ON (L90 OR L91) AND L10
D SCAN
SAVE TEMP L92 KUM327CRX1B/A

FILE 'CHEMINFORMRX' ENTERED AT 10:03:05 ON 23 AUG 2006
L93 43 SEA SSS SAM L79 (304 REACTIONS)

FILE 'STNGUIDE' ENTERED AT 10:04:06 ON 23 AUG 2006
D SAVED

FILE 'ZCAPLUS' ENTERED AT 10:40:34 ON 23 AUG 2006
L94 QUE ABB=ON PLU=ON C07F001-02/IPC
L95 QUE ABB=ON PLU=ON C07B?/IPC
L96 QUE ABB=ON PLU=ON (C07B041 OR C07B043 OR C07B045)/IPC

FILE 'LWPI' ENTERED AT 10:42:02 ON 23 AUG 2006
L97 QUE ABB=ON PLU=ON ((N261 OR N262 OR N263) (P) (N341 OR N342 OR
N343 OR N331 OR N332 OR N333 OR N334 OR N335 OR N352))/M0,M1,M2
,M3,M4,M5,M6

FILE 'USPATFULL, USPAT2' ENTERED AT 10:43:52 ON 23 AUG 2006
L98 5394 SEA ABB=ON PLU=ON L63 OR L64
L99 5 SEA ABB=ON PLU=ON L98 AND L18
L100 55 SEA ABB=ON PLU=ON L98 AND L16/TI,IT,CC,CT,ST,STP
L101 59 SEA ABB=ON PLU=ON L98 AND L14/TI,IT,CC,CT,ST,STP
L102 135 SEA ABB=ON PLU=ON L14/TI,IT,CC,CT,ST,STP AND L16/TI,IT,CC,CT,
ST,STP
L103 234 SEA ABB=ON PLU=ON (L99 OR L100 OR L101 OR L102) AND L11
L104 137 SEA ABB=ON PLU=ON L103 AND L19/TI,IT,CC,CT,ST,STP,BI,AB
L105 26 SEA ABB=ON PLU=ON L103 AND L12/TI,IT,CC,CT,ST,STP,BI,AB
L106 14 SEA ABB=ON PLU=ON L103 AND L13/TI,IT,CC,CT,ST,STP,BI,AB
L107 8 SEA ABB=ON PLU=ON L104 AND L105 AND L106
D SCAN
L108 7 SEA ABB=ON PLU=ON L103 AND L94
L109 10 SEA ABB=ON PLU=ON L103 AND (L95 OR L96)
L110 16 SEA ABB=ON PLU=ON (L108 OR L109) AND L11
L111 22 SEA ABB=ON PLU=ON L107 OR L110
L112 1 SEA ABB=ON PLU=ON L103 AND L96
L113 1 SEA ABB=ON PLU=ON L108 AND L112
L114 1 SEA ABB=ON PLU=ON L108 AND L109
L115 8 SEA ABB=ON PLU=ON L107 OR (L112 OR L113 OR L114)
L116 8 SEA ABB=ON PLU=ON L115 AND L11
SAVE TEMP L116 KUM327USP1B/A

FILE 'STNGUIDE' ENTERED AT 10:49:38 ON 23 AUG 2006

FILE 'WPIX' ENTERED AT 10:49:43 ON 23 AUG 2006
SELECT L2 1- DCRE
L117 0 SEA ABB=ON PLU=ON 71660-0-0-0/DSCE
L118 1 SEA ABB=ON PLU=ON 71660-0-0-0/DCSE
D SCAN
SELECT L2 1- DCN
L119 1 SEA ABB=ON PLU=ON (RADROW/SDCN OR 0126-86201/SDCN OR
0126-86202/SDCN OR 0126-86203/SDCN OR 0126-86204/SDCN OR
0126-86205/SDCN)
D SCAN
D QUE STAT L62
L120 0 SEA SSS SAM L60
D QUE STAT
L121 0 SEA SSS FUL L60
L122 22 SEA ABB=ON PLU=ON L97 AND L94
D TRI 1-5
L123 19 SEA ABB=ON PLU=ON L122 AND ((DEPROTON?/BIX OR (DE/BIX(W)PROTO
N?/BIX)) OR (ELECTROPHIL?/BIX OR (ELECTRO/BIX(W)PHIL?/BIX)) OR

(COUPLING/BIX) OR (LITHIUM/BIX OR LI/BIX) OR (LITHIAT?/BIX OR LITHIUMIZ?/BIX OR LITHIZE?/BIX) OR ((CARBON/BIX(4A) (N/BIX OR O/BIX OR S/BIX OR P/BIX OR NITROGEN/BIX OR OXYGEN/BIX OR SULFUR/BIX OR SULPHUR/BIX OR PHOSPHORUS/BIX OR HETEROATOM/BIX OR (HETERO/BIX(W)ATOM/BIX))) (7A) (BOND?/BIX OR ATTACH?/BIX OR LINK?/BIX)) OR (ORGANOLITH?/BIX OR (ORGANO/BIX(W)LITH?/BIX) OR (ORGANIC/BIX(W)LITH?/BIX)) OR (ARYLLITH?/BIX OR ALKYLLITH?/BIX OR METHYLLITH?/BIX OR ETHYLLITH?/BIX OR PROPYLLITH?/BIX OR BUTYLLITH?/BIX OR ((ARYL/BIX OR ALKYL/BIX OR METHYL/BIX OR ETHYL/BIX OR PROPYL/BIX OR BUTYL/BIX) (W) (LI/BIX OR LITH?/BIX)))

L124 22 SEA ABB=ON PLU=ON L122 OR L123
 D TRI 1-5
 D IBIB 1-4
 SAVE TEMP L124 KUM327WPI1B/A
 L125 6 SEA ABB=ON PLU=ON (L5 OR L6 OR L7 OR L8) AND L94
 L126 13 SEA ABB=ON PLU=ON (L5 OR L6 OR L7 OR L8) AND L97
 L127 8 SEA ABB=ON PLU=ON (L5 OR L6 OR L7 OR L8) AND L96
 L128 2 SEA ABB=ON PLU=ON L125 AND (L126 OR L127)
 L129 2 SEA ABB=ON PLU=ON L125 AND L126
 L130 7 SEA ABB=ON PLU=ON L126 AND L127
 L131 7 SEA ABB=ON PLU=ON L128 OR L130
 SAVE TEMP L131 KUM327WPIINV/A
 L132 0 SEA ABB=ON PLU=ON L2 NOT L131

FILE 'STNGUIDE' ENTERED AT 11:02:05 ON 23 AUG 2006

FILE 'MEDLINE, BIOSIS, EMBASE' ENTERED AT 11:02:28 ON 23 AUG 2006

L133 126 SEA ABB=ON PLU=ON L65 OR L66 OR L67
 L134 2 SEA ABB=ON PLU=ON L133 AND (L19 OR L14)
 L135 3 SEA ABB=ON PLU=ON L133 AND L16
 L136 6 SEA ABB=ON PLU=ON L133 AND (L12 OR L13)
 L137 9 SEA ABB=ON PLU=ON (L134 OR L135 OR L136)
 D SCAN
 D QUE
 SAVE TEMP L137 KUM327MULS/A

FILE 'STNGUIDE' ENTERED AT 11:04:29 ON 23 AUG 2006

D SAVED

FILE 'MEDLINE, BIOSIS, EMBASE, PASCAL, JICST-EPLUS, JAPIO, CABA, LIFESCI, BIOENG, BIOTECHNO, BIOTECHDS, DRUGU, DRUGB, VETU, VETB, SCISEARCH, CONFSCI, DISSABS' ENTERED AT 11:06:11 ON 23 AUG 2006

L138 1521 SEA ABB=ON PLU=ON (L5 OR L6 OR L7 OR L8 OR L9)
 L139 1 SEA ABB=ON PLU=ON L138 AND (L16 OR L38 OR L41)
 L140 19 SEA ABB=ON PLU=ON L138 AND L17
 L141 1 SEA ABB=ON PLU=ON (L139 OR L140) AND (L12 OR L13 OR L19)
 D SCAN
 SAVE TEMP L141 KUM327MULINV/A
 L142 3180 SEA ABB=ON PLU=ON (L17 OR L16 OR L38 OR L41) (20A) (L19 OR L14)
 L143 49 SEA ABB=ON PLU=ON L142 AND L12
 L144 13 SEA ABB=ON PLU=ON L143 AND L13
 D SCAN
 L145 7 SEA ABB=ON PLU=ON L144 AND L10
 SAVE TEMP L145 KUM327MUL1B/A
 D SAVED

FILE 'STNGUIDE' ENTERED AT 11:22:53 ON 23 AUG 2006

D QUE STAT L25

D QUE STAT L62
D QUE NOS L58
D QUE NOS L78
D QUE STAT L80
D QUE NOS L92
D QUE STAT L93
D QUE NOS L116
D QUE STAT L121
D QUE L124
D QUE NOS L137
D QUE L145

FILE 'HCAPLUS, CASREACT, USPATFULL, USPAT2, WPIX, MEDLINE, BIOSIS,
EMBASE, SCISEARCH, DISSABS' ENTERED AT 11:25:37 ON 23 AUG 2006
L146 115 DUP REM L78 L58 L92 L116 L124 L137 L145 (75 DUPLICATES REMOVED)
ANSWERS '1-71' FROM FILE HCAPLUS
ANSWERS '72-74' FROM FILE CASREACT
ANSWERS '75-81' FROM FILE USPATFULL
ANSWERS '82-101' FROM FILE WPIX
ANSWER '102' FROM FILE MEDLINE
ANSWERS '103-111' FROM FILE BIOSIS
ANSWER '112' FROM FILE SCISEARCH
ANSWERS '113-115' FROM FILE DISSABS

FILE 'STNGUIDE' ENTERED AT 11:25:47 ON 23 AUG 2006

FILE 'HCAPLUS, CASREACT, USPATFULL, WPIX, MEDLINE, BIOSIS, SCISEARCH,
DISSABS' ENTERED AT 11:26:22 ON 23 AUG 2006
D IBIB ED AB HITIND HITSTR

FILE 'STNGUIDE' ENTERED AT 11:26:24 ON 23 AUG 2006

FILE 'HCAPLUS, CASREACT, USPATFULL, WPIX, MEDLINE, BIOSIS, SCISEARCH,
DISSABS' ENTERED AT 11:26:45 ON 23 AUG 2006
D IBIB ED AB HITIND HITSTR 2-71

FILE 'STNGUIDE' ENTERED AT 11:26:59 ON 23 AUG 2006

FILE 'HCAPLUS, CASREACT, USPATFULL, WPIX, MEDLINE, BIOSIS, SCISEARCH,
DISSABS' ENTERED AT 11:28:05 ON 23 AUG 2006
D IBIB ED AB FHIT 72

FILE 'STNGUIDE' ENTERED AT 11:28:11 ON 23 AUG 2006

FILE 'HCAPLUS, CASREACT, USPATFULL, WPIX, MEDLINE, BIOSIS, SCISEARCH,
DISSABS' ENTERED AT 11:28:37 ON 23 AUG 2006
D IBIB AB FHIT 73-74

FILE 'STNGUIDE' ENTERED AT 11:29:00 ON 23 AUG 2006

FILE 'HCAPLUS, CASREACT, USPATFULL, WPIX, MEDLINE, BIOSIS, SCISEARCH,
DISSABS' ENTERED AT 11:29:21 ON 23 AUG 2006
D IBIB AB HITSTR 75-81

FILE 'STNGUIDE' ENTERED AT 11:29:22 ON 23 AUG 2006

FILE 'HCAPLUS, CASREACT, USPATFULL, WPIX, MEDLINE, BIOSIS, SCISEARCH,
DISSABS' ENTERED AT 11:30:25 ON 23 AUG 2006
D IALL ABEQ TECH ABEX 82-101

FILE 'STNGUIDE' ENTERED AT 11:30:38 ON 23 AUG 2006

FILE 'HCAPLUS, CASREACT, USPATFULL, WPIX, MEDLINE, BIOSIS, SCISEARCH,
DISSABS' ENTERED AT 11:32:03 ON 23 AUG 2006
D IBIB ED AB IND 102-115

FILE 'STNGUIDE' ENTERED AT 11:32:07 ON 23 AUG 2006
D QUE L40
D QUE L131
D QUE L141

L147 FILE 'HCAPLUS, WPIX, JAPIO' ENTERED AT 11:33:36 ON 23 AUG 2006
10 DUP REM L40 L131 L141 (2 DUPLICATES REMOVED)
ANSWERS '1-4' FROM FILE HCAPLUS
ANSWERS '5-9' FROM FILE WPIX
ANSWER '10' FROM FILE JAPIO

FILE 'STNGUIDE' ENTERED AT 11:33:45 ON 23 AUG 2006

FILE 'HCAPLUS, WPIX, JAPIO' ENTERED AT 11:33:52 ON 23 AUG 2006
D IBIB ED AB 1-10

FILE 'STNGUIDE' ENTERED AT 11:33:58 ON 23 AUG 2006

FILE HOME

FILE ZCAPLUS

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FILE COVERS 1907 - 23 Aug 2006 VOL 145 ISS 9
FILE LAST UPDATED: 22 Aug 2006 (20060822/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE HCAPLUS

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FILE COVERS 1907 - 23 Aug 2006 VOL 145 ISS 9

FILE LAST UPDATED: 22 Aug 2006 (20060822/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Aug 18, 2006 (20060818/UP).

FILE WPIX

FILE LAST UPDATED: 22 AUG 2006 <20060822/UP>

MOST RECENT DERWENT UPDATE: 200654 <200654/DW>

DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,
PLEASE VISIT:

http://www.stn-international.de/training_center/patents/stn_guide.pdf <

>>> FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE
<http://scientific.thomson.com/support/patents/coverage/latestupdates/>

>>> PLEASE BE AWARE OF THE NEW IPC REFORM IN 2006, SEE
http://www.stn-international.de/stndatabases/details/ipc_reform.html and
<http://scientific.thomson.com/media/scpdf/ipcrdwpi.pdf> <<<

>>> FOR FURTHER DETAILS ON THE FORTHCOMING DERWENT WORLD PATENTS
INDEX ENHANCEMENTS PLEASE VISIT:

http://www.stn-international.de/stndatabases/details/dwpi_r.html <<<

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 21 AUG 2006 HIGHEST RN 903048-34-0

DICTIONARY FILE UPDATES: 21 AUG 2006 HIGHEST RN 903048-34-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

FILE LREGISTRY

LREGISTRY IS A STATIC LEARNING FILE

NEW CAS INFORMATION USE POLICIES, ENTER HELP USAGETERMS FOR DETAILS.

FILE CASREACT

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FILE CONTENT:1840 - 20 Aug 2006 VOL 145 ISS 8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*      CASREACT now has more than 10 million reactions
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE CHEMINFORMRX
FILE LAST UPDATED: 12 JUN 2006 <20060612/UP>

>>> CAS Registry Numbers are available for
substances prior to 1995 <<<

FILE LWPI
LWPI IS A STATIC LEARNING FILE
>>> PATENT DRAWINGS AVAILABLE FOR DISPLAY <<<

FILE USPATFULL
FILE COVERS 1971 TO PATENT PUBLICATION DATE: 22 Aug 2006 (20060822/PD)
FILE LAST UPDATED: 22 Aug 2006 (20060822/ED)
HIGHEST GRANTED PATENT NUMBER: US7096505
HIGHEST APPLICATION PUBLICATION NUMBER: US2006185050
CA INDEXING IS CURRENT THROUGH 22 Aug 2006 (20060822/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 22 Aug 2006 (20060822/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2006
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2006

FILE USPAT2

FILE COVERS 2001 TO PUBLICATION DATE: 22 Aug 2006 (20060822/PD)
FILE LAST UPDATED: 22 Aug 2006 (20060822/ED)
HIGHEST GRANTED PATENT NUMBER: US2006126039
HIGHEST APPLICATION PUBLICATION NUMBER: US2006185040
CA INDEXING IS CURRENT THROUGH 22 Aug 2006 (20060822/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 22 Aug 2006 (20060822/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2006
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2006

FILE MEDLINE

FILE LAST UPDATED: 22 Aug 2006 (20060822/UP). FILE COVERS 1950 TO DATE.

On December 11, 2005, the 2006 MeSH terms were loaded.

The MEDLINE reload for 2006 is now (26 Feb.) available. For details on the 2006 reload, enter HELP RLOAD at an arrow prompt (=>).

See also:

<http://www.nlm.nih.gov/mesh/>
http://www.nlm.nih.gov/pubs/techbull/nd04/nd04_mesh.html
http://www.nlm.nih.gov/pubs/techbull/nd05/nd05_med_data_changes.html
http://www.nlm.nih.gov/pubs/techbull/nd05/nd05_2006_MeSH.html

OLDMEDLINE is covered back to 1950.

MEDLINE thesauri in the /CN, /CT, and /MN fields incorporate the MeSH 2006 vocabulary.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE BIOSIS

FILE COVERS 1969 TO DATE.

CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNS) PRESENT
FROM JANUARY 1969 TO DATE.

RECORDS LAST ADDED: 17 August 2006 (20060817/ED)

FILE EMBASE

FILE COVERS 1974 TO 23 Aug 2006 (20060823/ED)

EMBASE has been reloaded. Enter HELP RLOAD for details.

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE PASCAL

FILE LAST UPDATED: 21 AUG 2006 <20060821/UP>

FILE COVERS 1977 TO DATE.

>>> SIMULTANEOUS LEFT AND RIGHT TRUNCATION IS AVAILABLE
IN THE BASIC INDEX (/BI) FIELD <<<

FILE JICST-EPLUS

FILE COVERS 1985 TO 22 AUG 2006 (20060822/ED)

THE JICST-EPLUS FILE HAS BEEN RELOADED TO REFLECT THE 1999 CONTROLLED TERM (/CT) THESAURUS RELOAD.

FILE JAPIO

FILE LAST UPDATED: 3 APR 2006 <20060403/UP>

FILE COVERS APRIL 1973 TO DECEMBER 22, 2005

>>> GRAPHIC IMAGES AVAILABLE <<<

>>> NEW IPC8 DATA AND FUNCTIONALITY NOT YET AVAILABLE IN THIS FILE.
USE IPC7 FORMAT FOR SEARCHING THE IPC. WATCH THIS SPACE FOR FURTHER
DEVELOPMENTS AND SEE OUR NEWS SECTION FOR FURTHER INFORMATION
ABOUT THE IPC REFORM <<<

FILE CABA

FILE COVERS 1973 TO 3 Aug 2006 (20060803/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

The CABA file was reloaded 7 December 2003. Enter HELP RLOAD for details.

FILE LIFESCI

FILE COVERS 1978 TO 16 Aug 2006 (20060816/ED)

FILE BIOENG

FILE LAST UPDATED: 16 AUG 2006 <20060816/UP>

FILE COVERS 1982 TO DATE

>>> SIMULTANEOUS LEFT AND RIGHT TRUNCATION AVAILABLE IN
THE BASIC INDEX <<<

FILE BIOTECHNO

FILE LAST UPDATED: 7 JAN 2004 <20040107/UP>

FILE COVERS 1980 TO 2003.

>>> BIOTECHNO IS NO LONGER BEING UPDATED AS OF 2004 <<<

>>> SIMULTANEOUS LEFT AND RIGHT TRUNCATION AVAILABLE IN
/CT AND BASIC INDEX <<<

FILE BIOTECHDS

FILE LAST UPDATED: 23 AUG 2006 <20060823/UP>

FILE COVERS 1982 TO DATE

>>> USE OF THIS FILE IS LIMITED TO BIOTECH SUBSCRIBERS <<<

FILE DRUGU

FILE LAST UPDATED: 21 AUG 2006 <20060821/UP>

>>> DERWENT DRUG FILE (SUBSCRIBER) <<<

>>> FILE COVERS 1983 TO DATE <<<

>>> THESAURUS AVAILABLE IN /CT <<<

FILE DRUGB

>>> FILE COVERS 1964 TO 1982 - CLOSED FILE <<<

FILE VETU

FILE LAST UPDATED: 02 JAN 2002 <20020102/UP>

FILE COVERS 1983-2001

FILE VETB

FILE LAST UPDATED: 25 SEP 94 <940925/UP>

FILE COVERS 1968-1982

FILE SCISEARCH

FILE COVERS 1974 TO 19 Aug 2006 (20060819/ED)

SCISEARCH has been reloaded, see HELP RLOAD for details.

FILE CONFSCI

FILE COVERS 1973 TO 10 Jul 2006 (20060710/ED)

CSA has resumed updates, see NEWS FILE

FILE DISSABS
FILE COVERS 1861 TO 27 JUL 2006 (20060727/ED)

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